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INTRODUCTION

The Institute for Computer Applications in Science and Engineering (ICASE)* is operated at the Langley Research Center (LaRC) of NASA by the Universities Space Research Association (USRA) under a contract with the Center. USRA is a nonprofit consortium of major U. S. colleges and universities.

The Institute conducts unclassified basic research in applied mathematics, numerical analysis and algorithm development, fluid mechanics, and computer science in order to extend and improve problem-solving capabilities in science and engineering, particularly in the areas of aeronautics and space research.

ICASE has a small permanent staff. Research is conducted primarily by visiting scientists from universities and industry who have resident appointments for limited periods of time as well as by visiting and resident consultants. Members of NASA's research staff may also be residents at ICASE for limited periods.

The major categories of the current ICASE research program are:

- Applied and numerical mathematics, including multidisciplinary design optimization;
- Theoretical and computational research in fluid mechanics in selected areas of interest to LaRC, such as transition, turbulence, combustion, and acoustics;
- Applied computer science: system software, systems engineering, and parallel algorithms.

ICASE reports are considered to be primarily preprints of manuscripts that have been submitted to appropriate research journals or that are to appear in conference proceedings. A list of these reports for the period April 1, 1995 through September 30, 1995 is given in the Reports and Abstracts section which follows a brief description of the research in progress.

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RESEARCH IN PROGRESS

APPLIED AND NUMERICAL MATHEMATICS

SAUL ABARBANEL

Error bounded algorithms for the diffusion and advection diffusion eqs. in 2-D

The SAT method for imposing b.c.'s such that the spatial finite differencing operator becomes negative definite, has been applied in the past to the case of 1-D diffusion equation solved via an explicit 4th order central-differencing. The 1-D case assumed that the end points do not necessarily correspond to node points.

This allows a direct, though not trivial, extension to the multi-dimensional case with a cartesian mesh. This idea was programmed and ran for the "complex" shape of a circle with a hole placed off center.

For a truly time dependent problem there are geometric parameters (*i.e.*, hole diameter and/or placement) that cause the standard method (with Dirichlet boundary conditions) to fail completely. The SAT method produced results with a bounded error as predicted.

It is planned to extend the same idea first to the case of multi-dimensional advection-diffusion problems and later to systems of such equations.

This work was conducted in collaboration with A. Ditkowski.

EYAL ARIAN

Multigrid methods for optimization problems

The motivation of this project is to develop efficient numerical methods to solve large scale optimization problems which are governed by PDE.

The approach is to use multigrid methods by representing the optimization problem on a set of grids with increasing level of refinement. The multigrid one-shot optimization method was extended to the infinite dimensional design space and applied numerically to optimal shape design problems which are governed by an elliptic PDE. An essential determinant for such an algorithm to converge is the smoothing property of the minimization process. Textbook multigrid convergence rates were achieved for optimal shape design in 2D governed by Poisson equation. This work was done in collaboration with S. Ta'asan.

Future plans include the extension of this work to aerodynamics shape optimization problems governed by full-potential and Euler equations, *i.e.*, efficient solvers for the infinite dimensional design case.

Analysis of the Hessian for aerodynamics optimization

Efficient solvers for optimization problems use Hessian information. This work is concerned with the analysis of the eigenvalue distribution for Hessians resulting from optimal shape design

problems governed by flow equations. The goal is to construct efficient preconditioners for such problems.

Analysis of Hessians for inviscid aerodynamics optimization problems has been done. Both the full potential and Euler equations were analyzed in two and three dimensions. The analysis shows that the Hessians for the matching pressure problem using the Full-Potential or Euler equations are identical. On the other hand, the optimization problem in two and three dimensions are inherently different. In three dimensions oscillation in the span-wise direction can develop and therefore a regularization of the shape in the span-wise direction is required. The choice of regularization parameters is determined by the analysis. The analysis also suggests an infinite dimensional preconditioner which is based on an infinite dimensional approximation for the Hessian, and can be applied using projections to finite dimensional design space.

Future plans include extension of the analysis to viscous flow. This work was done in collaboration with S. Ta'asan.

Aeroelastic optimization problems

The objective of this work is to develop tools that will enable the construction of efficient numerical algorithms to solve aeroelastic optimization problems.

The small-disturbance shape optimization of a $2D$ isotropic flat plate under $3D$ full-potential flow was analyzed. The symbol of the Hessian near the minimum of the cost function (pressure matching) was computed. The analysis show that the aerodynamics block in the Hessian is ill-conditioned while the structure block is well-conditioned. From the analysis it is possible to determine a preconditioner which will give a good approximation of the inverse of the Hessian for the coupled system. However, the analysis show that the coupling in this system is not strong and therefore a serial algorithm in which the shape is optimized relative to aerodynamics considerations only, followed by structural optimization limited to a given shape should converge to the optimal solution in a few multidisciplinary iterations.

Future plans include numerical implementation of the above preconditioner in an optimization algorithm.

Preconditioning of MDO problems

In general, it is likely that MDO problems are going to have at least two disciplines which are strongly coupled. The aim of this research project is to develop efficient optimization algorithms to solve such problems.

The approach is to use local mode analysis to develop preconditioners for the strongly coupled disciplines. Preliminary numerical results have been obtained for a simple model problem composed of two strongly coupled systems governed by Poisson equations. The results of applying the above preconditioners show a very fast convergence rate in comparison to a serial algorithm in which each disciplinary optimization problem is optimized using the disciplinary gradients only.

Future plans include numerical implementation to nonlinear MDO problems.

CHRISTINA L. BLOEBAUM

Optimal sequencing of complex systems for parallel implementation

Multidisciplinary Design Optimization (MDO) problems are typical of complex engineering systems in which participating subsystems are coupled through transference of output data. The couplings imply an iterative solution approach that can be extremely computationally expensive. It is therefore advantageous to have the ability to sequence the participating modules in such a way as to minimize a functional that represents the designer's objective. This may be, for example, to minimize computational time or cost associated with converging the complex system.

Opportunities for exploiting inherent parallelism during sequencing were explored in this work. Use of a Genetic Algorithm (GA) was explored to maximize possibilities of implementing a distributed processing convergence scheme (PVM - Parallel Virtual Machine - was investigated). Small sample non-hierarchic systems with minimal iterative feedbacks were initially used. An assumption of unlimited processors was assumed.

Continuing and further work include incorporating minimization of computational time associated with the critical path as a functional term for the GA. The approach will be applied to more complex systems to verify the validity of the optimal sequencing strategy.

JOHN A. BURNS

Approximation and analysis of optimization based design algorithms

The development of practical computational tools for design optimization can be approached from several directions. However, the construction of a useful computational algorithm will require that numerical approximations be introduced at some point in the design process. If viewed as infinite dimensional optimal control problems, then most optimal design methods fall somewhere between the *approximate-then-optimize (ATO)* paradigm and the *optimize-then-approximate (OTA)* approach. Black box methods are examples of the *ATO* approach. Black box methods are often achieved by cascading simulation software into optimization algorithms. Although the explicit form of the black box algorithm may vary, there is often the un-stated assumption that cascading a good simulation software into a good optimizer will produce a good optimal design algorithm. Except for some special cases involving the design of optimal control laws, there is almost no theoretical basis for this assumption and examples are known where this assumption is not valid. On the other hand *OTA* type approaches, such as one-shot and control theory methods, avoid this difficulty by directly approximating the (infinite dimensional) necessary conditions. However, these methods usually lead to a considerable increase in computational complexity. Both approaches have benefits and drawbacks.

The approach we are considering combines some of the advantages of the black box *ATO* type paradigms with optimal control *OTA* type approaches. The method uses numerical approximations of infinite dimensional sensitivity equations to produce gradient information for a discretized optimization problem. The resulting sensitivity equation method (SEM) eliminates the need to compute grid sensitivities in shape optimization problems. However, this algorithm does not always produce consistent gradients and hence it becomes important to select a robust optimization algorithm. We have investigated several standard numerical schemes used to simulate nonlinear conservation

equations and shown that the SEM will produce consistent gradients when these schemes are combined properly. These results allowed us to develop a convergence theory for optimization based design algorithms. We have tested these algorithms on various shape optimization problems and achieved excellent numerical results.

As noted above, some simulation schemes do not lead to consistent gradients and robust optimization is essential. We are developing a theoretical framework to address the basic convergence questions for this case. One approach relies on the concept of asymptotically consistent gradients. We plan to combine trust region methods with numerical schemes that produce asymptotically consistent gradients and show that the resulting SEM based design algorithm converges. The goal is to produce fast algorithms by taking advantage of certain high order simulation schemes that produce asymptotically consistent gradients of sufficient quality that they can be used by trust region optimization methods.

WEI CAI

Fast algorithms for electromagnetic field computations of microstrip antenna and VLSI chip

Development of fast algorithms for the electromagnetic field computations for multiple-stacked microstrip antenna and VLSI microchip performance simulations.

The computation of the electromagnetic fields of microstrip antenna and VLSI microchip can be reduced to a problem of solving a Fredholm integral equation of second kind. The solution of the integral equation by boundary element methods is then reduced to solving a full dense matrix equations. There are two major costs in this process, one is associated with the filling-in of the matrix entries, another is the solution of the dense matrix system.

We have made significant progress in resolving the first difficulty, namely, the filling-in of matrix entries. The difficulty with the matrix filling-in is that the Green's function for the general multi-layered medium in a microstrip antenna or a microchip is given by a Hankel transformation using complex contour integral. The integrand contains various unknown surface wave poles, which depend on the structure of the antenna or microchip, and demonstrate oscillatory decay at the infinite. We have successfully applied our *wavelet approximation* to overcome the singularities caused by the poles and, at the same time, constructed a unique *spectral method* to overcome the oscillatory decays of the integrand.

We plan to test the developed numerical methods on various kinds of antenna and microchip configurations. Meanwhile, we will also investigate how to develop fast solution algorithm for the dense matrix system.

SUKUMAR R. CHAKRAVARTHY

Analysis and extensions of methods that update cell averages and their moments or derivatives

In prior work, we have successfully developed methods based on multidimensional interpolation/reconstruction that are essentially nonoscillatory and higher than second order accuracy for any cell shape and grid topology. These were based on increasingly larger stencils which provided

the data necessary to fit higher order polynomials in order to evaluate their coefficients. The objective of the present effort is to seek similarly applicable methods that are more efficient and/or easier to implement.

In the last several years several researchers have introduced methods that are more localized. Rather than using wider stencils, they update the polynomial coefficients by deriving additional equations. The most popular method to obtain these is by taking moments of the original equation. A method that takes derivatives has also been attempted. In the commenced effort, the motivation is to analyze, evaluate, and extend such schemes as part of a quest for higher than second order methods that are more easy to implement and/or more efficient for application to h, h-p, and p refinement methods. This work is being done in collaboration with V. Venkatakrishnan.

We plan to synthesize ideas from finite element and finite volume literature to develop practical higher order discretizations for the solution of Navier-Stokes equations on unstructured grids.

TONY F. CHAN

Domain decomposition and multilevel preconditioners for elliptic problems on unstructured meshes

Recently, unstructured finite element meshes have become very popular in scientific computing, primarily because of their flexibility in adapting to complicated geometries and the resolution of fine scale structures in the solution. Since no natural coarser grids exist as in structured meshes, practical multilevel domain decomposition and multigrid algorithms must allow coarser grids which are non-quasi-uniform and with boundaries and interior elements which are not necessarily matching to that of the fine mesh. Therefore, traditional solvers have to be modified so that their efficiency will not be adversely affected by the lack of structure.

We have developed a general framework for convergence analyses applicable to unstructured meshes, which can be viewed as a natural extension of the one formulated by Xu [SIREV 92] for structured meshes. We have developed techniques for constructing a coarse grid hierarchy from the given fine grid, as well as mesh partitioning algorithms. We developed special treatments to correctly implement different types of boundary conditions. Our numerical results for domain decomposition and multigrid methods on unstructured meshes show convergence properties that are similar to those for standard structured meshes.

We plan to further develop both the theory and the algorithms for more general problems, including parabolic, convection diffusion and fluid flow problems. We'd also like to study convergence issues for agglomeration techniques which have the advantage of not requiring a coarse grid hierarchy.

JENNIFER M. DEANG

A computational study of numerical methods and solvers for the time dependent Ginzburg-Landau equations

My work was centered around a numerical study that included the implicit Euler method, a partial implicit Euler method, an explicit Euler method, and a Newton iteration method. All methods were used to solve the Time Dependent Ginzburg-Landau equations. Three-dimensions

calculations with the Newton method in conjunction with a direct solver were being very inefficient and a more efficient method was needed to achieve faster computational speed and less needed storage.

The Newton method can double the time step when the solution is not changing drastically at each time step which always occurs in steady state time evolution computations. But all of the Euler methods have one draw back: that the time step has to be sufficiently *small* and constant with these schemes. However, the implicit Euler method agreed very nicely with the time evolution solutions of the Newton method and had faster computational speed compared to the Newton method in terms of each time step due to a single matrix solve at each time step with Euler compared to several solves with the Newton method. This increase in speed at each time step was a trade off since the time step for the implicit Euler is small and constant while the Newton as stated before can be doubled in certain situations. On the other hand, the partial implicit and explicit Euler methods' outputs did not agree with the time evolution solutions from the Newton method even with very *small* restricted time steps.

The direct solver that was in use was no longer feasible to solve three dimensional problems on a workstation or even in parallel on several workstations. So iterative solvers were needed in order handle larger 3D domains in an effort to simulate experimental data. Several iterative solvers have been looked at but the subject of convergence of these iterative solvers has been very difficult to achieve in certain cases. On going research is being done in this area of combining one of the numerical methods mentioned above to an iterative solver in an effort to be able to solve on larger computational regions in a reasonable amount of computational time.

PAUL FISCHER

Projection techniques for computational fluid dynamics

Efficient solution of the Navier-Stokes equations in complex domains is dependent upon the availability of fast solvers for sparse linear systems. We seek to improve existing spectral element methods for free-surface flows through development of projection techniques for the the pressure and mesh solves.

Implicit or semi-implicit numerical treatment of time-dependent partial differential equations typically necessitates repeated solution of a particular set of sparse linear systems of equations. For evolving solutions, projection techniques can be an effective means to generating good approximations to the solution at the current time step, and thereby reduce the required effort for subsequent iterative solution of the linear system. We showed that projection techniques can yield a typical two- to four-fold reduction in CPU time for iterative-based solution of unsteady incompressible flows in fixed geometries. In the present work, we have applied these techniques to the mesh computation phase of free-surface calculations. The mesh is subject to the global constraint that it be volume preserving. The elasticity solver employed to enforce this constraint is solved iteratively at each time step, often requiring hundreds of matrix-vector products on a vector-valued field; the dimension of the linear system, n , is equal to the number of grid points times the spatial dimension, d ($d=2$ or 3). The projection is based upon l previous solutions, with $l_{\max} \simeq 20 - 40$. Unlike the static geometry case, the moving mesh implies that the linear systems are time dependent. Consequently, the basis set must be re-orthogonalized with respect to the inner-product based upon

the new system at each time step. To effect this via Gram-Schmidt orthogonalization requires l matrix-vector products and $l^2/2$ inner-products per time step.

Projection techniques for both the mesh and pressure solves have been incorporated into a spectral element based free-surface Navier-Stokes code. We have found that re-orthogonalization is important for the elasticity solver used for the mesh calculation. The pressure solve did not require re-orthogonalization, although the quality of the projection-based approximation did deteriorate rapidly unless the basis set was frequently refreshed ($l_{\max} \simeq 5$). With the basis re-orthogonalization for the mesh, and no re-orthogonalization for the pressure, a four-fold reduction in CPU time has been observed for computations of axisymmetric droplet-plate interactions involving several thousand grid points.

WILLIAM FOLLETT

Multidisciplinary optimization of aerospike rocket nozzles

The objective of this research is to investigate different optimization methodologies in the context of coupling CFD flowsolvers and FEM structures analysis to design an aerospace nozzle. To effectively design a rocket engine with good thrust to weight ratio characteristics, a methodology is required which can couple high fidelity design and analysis tools from various disciplines early in the design cycle to shorten development time and provide increased performance of the final product. Since some of these analysis tools can be computationally expensive to use, it is imperative that efficient multidisciplinary optimization methods are employed.

The effectiveness of several optimization methods were investigated using increasingly complex analysis methods as confidence in the process improved. Initially, a CFD surrogate model was constructed and used in place of CFD analysis to simulate the basic characteristics of a CFD nozzle solution including the effects of three design variables and numerical noise on the objective function. This was coupled to a simple analytic structural model for initial optimization studies which maximized the quantity (thrust/weight), while satisfying constraints corresponding to maximum stress, buckling and deflection limits. The performance of several optimization routines was evaluated for their effectiveness on this type of problem. Specifically, the generalized reduced gradient algorithm, sequential quadratic programming, simulated annealing, and implicit function filtering methods were tested. Additionally, parametric FEM and CFD models were constructed, coupled to optimization routines, and demonstrated individually.

The performance of optimization methods will be evaluated with the coupled FEM and CFD models. Also, surrogate modeling techniques such as neural nets, orthogonal arrays, and Bayesian validated models will be investigated to explore their potential for reducing the number of expensive CFD runs required. This work was conducted in conjunction with J. Korte (NASA Langley).

JAMES GEER

Periodic basis functions with built-in discontinuities

Series expansions of functions, such as Fourier series, perturbation series, etc., are often useful in developing numerical or semi-numerical, semi-analytical algorithms for the solution of differential equations. However, when only a partial sum of such a series is used, some “undesirable”

effects (such as the Gibbs phenomena) may be present, or the partial sum may have “difficulty” approximating certain features of the solution, such as boundary layers, internal layers, or various discontinuities.

For a certain class of function $f(x)$, the combination of a finite sum of certain periodic basis functions with “built-in” singularities, along with a finite Fourier series, leads to a sequence of approximations which converges *exponentially* to f in the *maximum norm*, even though f may have a finite number of discontinuities. In particular, these approximations eliminate the Gibbs phenomena. In order to implement this approach, a knowledge of the locations and magnitudes of the jumps in f and its derivatives is necessary. A highly robust method of estimating these quantities from a finite number of the Fourier coefficients of f using at least squares technique is being studied.

The class of basis functions with “built-in” singularities will be extended to include functions that have more general singularities, such as fractional power (e.g., square root) and logarithmic singularities. They will be applied to several model problems which either have discontinuities in the initial data and/or develop discontinuities (or “near-discontinuities”) as time increases.

An analysis of an acoustic/viscous splitting technique for computational aeroacoustics

Since Lighthill’s original “acoustic analogy” theory of aerodynamic noise generation, much effort has been devoted to the analysis and computation of sound generated by fluid flows. Only recently has enough computing power become available so that it is possible to consider the direct computation of sound fields from the fundamental governing equations, without the artifice of the analog approach.

The underlying philosophy of the approach being considered is that, at low Mach numbers, the sound radiated from a flow can be calculated readily using the viscous, incompressible flow as the forcing function in a linearized analysis. In short, a flow is first computed treating the fluid as *viscous* and *incompressible*, and then this flow is used to “force” a flow in which the fluid is treated as being *inviscid* and *slightly compressible*. An analysis of how these flows can best be coupled is the subject of this study. In particular, for flow with a small Mach number and a large Reynolds number, several versions of the multiple scale perturbation technique are being explored.

Different scaling of several different classes of problems need to be considered and analyzed. In each case, the coupling of the two flows dictated by the perturbation method will need to be analyzed from both a theoretical point of view and from a practical, computational point of view. In particular, the effects of neglecting viscosity in the slightly compressible flow will need to be quantified.

MAX GUNZBURGER

Feedback and optimal control of unsteady flows

Ongoing work is conducted to demonstrate the feasibility of control of 2-D Tollmien-Schlichting waves in boundary-layers. The short-range objective is to develop procedures to control the growth of general disturbances in two and three-dimensional boundary-layers to delay transition. Optimal control theory is also used to determine the time-dependence of the controller input. The long-range

objective is to develop such methodologies for a wide variety of flow problems including separation control in high-lift configurations.

Tollmien-Schlichting waves (TS) are introduced into a Blasius boundary layer. The nonlinear incompressible Navier-Stokes equations are then solved by DNS using a combination of spectral and high-order finite-difference methods. The growth rate of the (TS) waves is reduced by superposition of a secondary wave of approximately equal amplitude, and 180° out of phase. Two closely spaced sensors located upstream of the input location of the secondary wave (which is input via blowing/suction) are necessary to determine phase and frequency of the existing wave. This is accomplished by computing the largest Fourier coefficient of the energy spectrum measured at one of the sensors.

The second component of this research used optimal control theory to produce the optimum time-dependent amplitude of a sinusoidal (in space) blowing and suction profile in the slot through which the secondary wave is input into the boundary-layer. The objective was to minimize the normal shear stress at a downstream sensor, over several periods of the TS wave. The solution to the resulting set of equations involved solving the Navier-Stokes equations in the downstream direction, and the adjoint system in the upstream direction.

Both methods demonstrate the feasibility of reducing the growth of the TS waves. The first, active method, produced almost exact cancelation of the TS wave since the frequency and amplitude of the TS wave were approximately known. It was conclusively demonstrated that it is indeed wave cancelation and not some other phenomenon that produced this cancelation. The optimal control theory resulted in a blowing/suction profile which degenerated in a perfect wave cancelation as the time control was applied was increased.

The next step in our research program will be to control three-dimensional boundary-layers on a swept wing, again with the aim of suppressing instabilities. We will also start to apply our methodology to other problems where flow control may be useful. For example, we will look flow separation and other problems related to high-lift configurations.

DAVID GOTTLIEB

Infiltration processes in material sciences

We are looking at the mathematical modeling and computations of infiltration processes in material sciences. In particular we try to model and analyze CVI processes (Chemical Vapor Infiltration processes).

We came with a simple system of two equations one for the solid phase and one for the fluid phase. The system is nonlinear but we were able to prove existence and uniqueness of the solution up to the time when the process terminates.

We have also formulated an optimization problem that its solution minimizes the time it takes the process to settle.

ANGELO IOLLO

Optimal shape design using the Euler equations

Faster computers and reliable numerical simulations make feasible some of the aerodynamics optimum design problems which are of engineering interest. The statement above becomes only partially true when we consider either flows governed by Euler or Navier-Stokes equations, or complicated geometrical configurations with many control parameters. For such cases, shape optimization seems to be still not practical due to extremely time consuming computation. The present work aims at a flexible and feasible approach for such intensive computational problems by applying the pseudo-time algorithm proposed by Shlomo Ta'asan. The algorithm consists of marching on the design hypersurface while improving the distance to the state and costate hypersurfaces. We consider the problem of matching the pressure distribution relative to a desired one, subject to the Euler equations, both for subsonic and supersonic flows. The rate of convergence to the minimum for the cases considered is 3 to 4 times slower compared to that of a single analysis. Results have been found for Ringleb flow and a shockless recompression case.

Further work includes three-dimensional Euler and two-dimensional Navier-Stokes test cases. This research is presently conducted in collaboration with M.D. Salas (NASA Langley) and S. Ta'asan (Carnegie Mellon University).

MICHAEL KOKKOLARAS

Enhanced simultaneous aerodynamic analysis and design optimization

Simultaneous Aerodynamic Analysis and Design Optimization (SAADO) is a technique which incorporates design improvement within the aerodynamic analysis in order to gain computational efficiency when the method of analysis is iterative. Both geometric and nongeometric parameters can be treated as design variables. In airfoil shape design, the variables are geometric. An interesting nongeometric variables application is the correction of experimental data obtained from wind tunnel measurements. Such measured data may include small errors due to wall interference and therefore do not agree with data obtained by numerical simulation from CFD codes using so called "free-air" boundary conditions.

The main idea here is to use the wind tunnel freestream conditions and parameters (Mach and Reynolds numbers, angle of attack, etc.) as initial conditions in a "free-air" code simulation and pose the optimization problem of matching the aerodynamic coefficients that were measured in the tunnel. The design, or optimization, variables of this problem are the parameters that one wishes to correct, usually the Mach number and the angle of attack. The enhancement to SAADO is incorporation of the pseudo-time, reduced optimization method of S. Ta'asan into existing codes. ANSERS, an implicit two-dimensional Navier-Stokes code based on an upwind, cell-centered, finite volume formulation is the analysis code and uses the Baldwin-Lomax model to simulate turbulence. The automatic differentiation tool ADIFOR is used in conjunction with an incremental iterative strategy to obtain the required sensitivity derivatives. As a first step, the single design variable (namely, the angle of attack α) problem has been solved, although not as efficiently as possible.

Future work focuses on the efficient solution of both the single and the two design variable problem, where the Mach number M is the second design variable. This work has benefited from

the appreciated guidance and help of P. Newman (NASA Langley), G. Hou (ICASE & ODU), and A. Taylor (ODU).

DAVID A. KOPRIVA

Spectral multidomain methods for compressible flows

We are developing a flexible quadrilateral based multidomain spectral method for the solution of both viscous and inviscid compressible flows. The main feature of the method is that internal to each subdomain, a staggered grid is used. At boundaries and subdomain interfaces, only the fluxes are defined. Solution unknowns are defined on a Gauss grid, and so are defined interior to subdomains. The inherent flexibility of the method comes from two facts: Only the flux is required to be continuous at an interface, and the fully staggered grid does not include subdomain corners.

For inviscid problems we have developed a fully non-conforming interface procedure. The requirement that the fluxes be continuous at an interface was relaxed, and instead the jump in the fluxes is required only to be orthogonal to the approximation space. The interface condition is implemented by a mortar method, where the Riemann problem for computing the flux is solved on the mortar. With the introduction of the fully non-conforming approximation, an inviscid solution can now be computed to spectral accuracy on an arbitrary tiling by quadrilaterals of a physical domain. We have also extended the inviscid conforming method to the solution of the compressible Navier-Stokes equations. In this case, the continuity of the normal viscous flux is enforced weakly. As before, the method does not include subdomain corners. The result is a method is flexible and easy to apply within the constraints of a conforming grid method. The method has been applied to a number of linear model problems in addition to the compressible Navier-Stokes equations themselves.

The next step is the application of the methods to time dependent problems. The interface treatment is formally accurate to the same order in time as the interior points. We will now examine the transparency of the interfaces to propagating waves. We will also consider the extension of the method for viscous problems to a non-conforming one.

MICHAEL LEWIS

Variable reduction approaches in problem formulation and nonlinear programming algorithms for MDO

The choice of problem formulation and nonlinear programming (NLP) algorithm can have a profound impact on the efficiency with which optimization problems can be solved. However, the complexity of problems governed by state constraints, which often arise in MDO and systems governed by differential equations, make it difficult to pursue multiple approaches to the solution of a problem based on varying degrees of variable elimination.

I developed an approach that allows one to practically pass between different problem formulations and NLP algorithms for their solution. As a practical concern, this approach requires a minimal amount of new code in order to try out a new variable reduction formulation. The key is first to implement the problem treating the state constraints purely as equality constraints; from this one can easily derive algorithms corresponding to alternative problem formulations.

This approach has already been tried on an elliptic inverse problem. I intend to develop a systematic implementation as part of my on-going work on the Nemo optimization software package.

The A. D. Welliver Program at the Boeing Co.

I spent most of the summer in Seattle visiting the Boeing Co. as an A. D. Welliver Fellow. This program, started this year, is intended primarily to expose university faculty to the business of a company such as Boeing so that engineering students might be better prepared in college. As a result of a conversation between P. Rubbert (Boeing) and M.Y. Hussaini, I was added to the list of participants with the idea that a person in basic research such as myself might come away with a much better focus on what research would help the needs of industry.

The program lasted eight weeks. The first week was devoted to overview and orientation; the last week was primarily for the academic participants to discuss ideas for changing the engineering curriculum, based on what was seen. The intervening six weeks were spent visiting all aspects of the Boeing Commercial Aircraft Group, from business acquisition and product development to product design and definition, production, and support.

I will give a presentation on what I saw at Boeing and the lessons I learned, as well as write a report on the experience.

JACQUES LIANDRAT

Wavelet based algorithm for PDE

Wavelet bases provide good space of approximation where PDE solution should be approached. However, to lead to efficient numerical methods, efficient approximation of linear and nonlinear operators must be available.

Based on basic properties of r -regular wavelets we proposed various algorithms for elliptic, parabolic, constant and non-constant coefficient linear operators. Numerical tests have been performed on the heat and Burgers equations in 1D and 2D with periodic boundary conditions.

Our directions of work are the approximation of nonlinear terms, the use of highly adapted spaces of approximation as well as implementations in complex configurations.

Signal approximation and modelization

Atomic decompositions related to wavelets are efficient to compress signals. They have not yet proven to be objectively efficient to model physics connected to the signals.

Various decompositions are being compared on a family of signals governed by simple model equations. In some cases models have been proposed and tested in more complex configuration such a laminar-turbulent transition or boundary layer turbulence signals.

A combined approximation of signals and governing operators will be defined using wavelet-like decompositions and should give access to finer physical modelization.

DIMITRI MAVRIPLIS

Unstructured multigrid techniques for the Navier-Stokes equations

The overall objective of this work is to develop efficient solution procedures for the Navier-Stokes equations on unstructured meshes involving low memory overhead and with eventual application to parallel machines.

The previously developed tetrahedral element based unstructured flow solver has been extended to enable the use of mixed-element meshes in two and three dimensions. In two dimensions, meshes consisting of mixed triangles and quadrilaterals can be handled, while in three dimensions meshes containing tetrahedra, prisms, pyramids and hexahedra may be employed. Block-structured meshes can also be handled by the present approach, simply by converting such meshes into a list of unstructured hexahedra. The various element types in the mesh can all be handled simultaneously by a single edge-based data-structure. The agglomeration multigrid algorithm, previously developed for tetrahedral meshes, has been generalized to meshes of arbitrary element types, and is used to accelerate convergence in the present scheme. Substantial computational savings have been demonstrated by employing hexahedral or prismatic elements over fully tetrahedral meshes, due to the lower connectivity (and hence lower number of edges) such elements incur. There is also evidence that a slightly higher accuracy may be achieved with such elements in certain regions of the flowfield. An automatic algorithm for combining simplicial elements (triangles in 2D, tetrahedra in 3D) into prismatic elements (or quadrilaterals in 2D) has been developed and demonstrated in the above context, in order to automatically reduce computational overheads for a given grid. This work has been conducted jointly with V. Venkatakrishnan.

A new effort has been initiated for improving the multigrid convergence rates of unstructured Navier-Stokes solvers. The main impediment to rapid convergence for these solvers is a result of the anisotropic nature of the problem, i.e. high grid stretching in the near wall and wake regions where boundary layers and wakes are expected. Based on the results of work previously carried out by Morano, Mavriplis and Venkatakrishnan, semi-coarsening or optimal coarsening strategies are being investigated as a means of improving the efficiency of the agglomeration multigrid technique for unstructured Navier-Stokes solvers.

BRIAN NGUYEN

Further works on bicharacteristic schemes for Maxwell's and the acoustics equations

The prediction of acoustic and electromagnetic wave scattering is used in the analysis of high speed circuits, radar cross-section and aircraft noise control, among others. Many such problems require long time propagation of waves, so dissipation and dispersion errors need to be kept small to maintain accurate solutions over the time of integration. To remove all dissipation errors, a leapfrog scheme is used, and to reduce dispersion errors, an upwind scheme is used.

We have completed the formal prediction of the second order upwind leapfrog scheme in two- and three-dimensions for both systems of equations, proving that the new scheme has better dispersion characteristics than Yee's central difference leapfrog scheme. An absorbing boundary condition for the bicharacteristic equations was also analyzed and tested, showing improved performances over

all known characteristic based absorbing boundary conditions. This work is conducted jointly with P. Roe.

The next step in this research is to further improve the accuracy of the scheme to fourth or higher order.

LUCA F. PAVARINO

Domain decomposition algorithms for first-order system least squares methods

New first-order system least squares methods have been recently proposed and analyzed for second order elliptic equations and systems. They produce symmetric and positive definite discrete systems by using standard finite element spaces which are not required to satisfy the inf-sup condition.

We have studied several domain decomposition algorithms for these first-order least squares methods. We have considered algorithms which are representative of the major classes of domain decomposition, i.e. overlapping and iterative substructuring algorithms, both in their additive and multiplicative variants. The theoretical and numerical results obtained show that the classical convergence bounds for standard Galerkin discretizations also hold for least squares methods.

Future research needs to be carried out for anisotropic coefficients and convection-diffusion problems.

Parallel spectral element preconditioners for linear elasticity

Standard finite element discretizations of the system of equations for linear elasticity suffer from the phenomenon of locking when the Poisson's ratio tends to $1/2$ (almost incompressible case). This problem can be overcome by using a mixed finite element formulation, at the price of obtaining a larger and indefinite linear system and having to choose carefully the finite element spaces in order to satisfy the inf-sup condition. Good parallel preconditioners for such systems are the key to the practical solution of large 3-D elasticity problems. While some work has been done for h-version finite elements, the problem is open for spectral and p-version finite elements.

In collaboration with O. Widlund (Courant Institute, NYU), we have studied and implemented a spectral element method for the mixed formulation of the system of 3-D linear elasticity. This method is analogous to the Q_P-Q_{p-2} spectral method of Maday, Patera and Ronquist for the Stokes system. We have designed domain decomposition preconditioners for both the whole indefinite system and the reduced Schur complement obtained by eliminating the interior variables. We are in the process of analyzing the convergence rate of our algorithms and their dependence on the spectral degree p , the number of subdomains N , and the Poisson's ratio ν .

Future work will try to extend these domain decomposition algorithms to the spectral element discretization of the Stokes system.

PETER G. PETROPOULOS

Analysis of finite diffraction gratings on dielectric interfaces

The Method of Matched Asymptotic Expansions is applied to the problem of plane wave scattering by a finite, but electrically large, periodic dielectric grating placed on the interface between two dielectric half-spaces. This work is being done in collaboration with G. Kriegsmann (NJIT).

A finite-difference code was debugged and validated for the problem of plane wave scattering by a dielectric square on wavelength at a side placed on the interface between two dielectric half-spaces. The validation was done by comparing the calculated radar cross-section with the one obtained by solving the same problem with an integral equation approach previously developed by us.

We plan to use the finite-difference code to solve for the cross-section of finite gratings up to 10 wavelengths long whose height and period are of the order of a wavelength in order to explore the accuracy of our approximate result.

JAGANNATHA RAO

Optimum topology design of discrete structures

It is well recognized that an optimal topology can impact the structural performance far more than just simple sizing or boundary shape optimization. However, the computation of optimal topologies remains one of the most difficult problem in applied optimization. In this project, our objective is to apply some of our recently developed new duality-based methods to a new class of problems, namely the topology design for eigenfrequency extremization in dynamic structures.

The basic new idea in this approach is to use the principles of duality to derive what we call the “design-variable-free design models,” i.e., design formulations from which the usual design variables (e.g., size and shape) have been eliminated, leaving behind only certain state variables (e.g., stress or strain fields). For the eigenvalue extremization problem, we have derived similar reduced models using the well-known concept of a dual matrix. As a first application, we have obtained new formulations in which a ground structure method is used to optimize the topology of vibration support structures.

Our next task is to numerically validate these new formulations. In particular, work is underway to implement a barrier type algorithm for the dual design problem; we will illustrate this new numerical capability by generating optimal topologies using very dense ground structures.

Game-theoretic formulations in MDO

Recently, we have had some success in applying the ideas from classical game theory to different mechanical design problems. In these problems, the principal characteristic was the simultaneous influence of more than one “designer” (or decision-maker or game player), each possessing only partial control over the final outcome. We feel that this ability to mathematically model multiple narrowly focussed “designers” can be extended to multiple disciplines as well. The objective in this project is to explore this idea further.

In game theory based approaches, the basic idea is to construct interacting or coupled mathematical models depending on the protocol existing between the different players such as, for

example, noncooperation, cooperation or even dominance (e.g., leader-follower relationship) over one another. In an MDO setting, so far we have developed an interesting but simple case study in the design of a cutting tool, the two disciplines here being the mechanics of metal cutting and the mechanics and costing of tool operation.

Next, we plan to construct game models for an actively controlled structure in which two disciplines, namely, the structures and the controls “players” will be modeled. Success in this more realistic MDO application will help us make the case that game-theoretic techniques can predict the final design outcome when different types of interdisciplinary interactions are permitted in a complex system.

PHILIP ROE

Multidimensional upwinding

The embodiment of physical modeling in a CFD code brings substantial advantages in terms of robustness and resolution even when this is done only through concepts of one-dimensional wave propagation. We continue a long-term project to incorporate more appropriate physical models of multidimensional flow.

As a result of work carried out this summer we have a better understanding of how our approach relates to other decompositions (Ta’asan) and to previous work on the Cauchy-Riemann problem (Brandt). It is also becoming clearer how our method extends to three dimensions. First multigrid results in two dimensions are encouraging.

We plan to concentrate in the immediate future on numerical approaches to the three-dimensional incompressible Euler equations, which contain both an elliptic component and a hyperbolic component (helicity). Although not further decomposable at the PDE level, there is still a possibility of treating the components distinctively at the discrete level.

Numerical methods for linear wave propagation

Linear waves occur in such important application areas as acoustics, electromagnetics, and elastodynamics. Within each area there is a frequent need to compute wave motion in the time domain involving propagation over many wavelengths. A class of methods without numerical dissipation and based on bicharacteristic analysis has been developed promising exceptional performance on coarse grids, and hence greatly reducing storage requirements.

It is desirable to keep the stencil of the scheme as compact as possible, both to improve overall accuracy and to retain that accuracy close to boundaries. We have developed fourth-order schemes on minimal stencils for both the acoustic and electromagnetic equations in two and three dimensions. Phase errors much smaller than one percent can be achieved with only four mesh points per wavelength.

In its current version, however, the three dimension version, as applied to electromagnetics, suffers an unstable mode and the immediate objective will be to remove this. Then the new algorithms will be applied to some practical problems in waveguide design.

CHI-WANG SHU

Discontinuous Galerkin method and shock vortex interaction

Our objective is to study and apply high order finite difference, finite elements and spectral methods for problems containing shocks. This will enable us to capture complicated flow structure over long period of time with a relatively coarse grid.

The investigation of the discontinuous Galerkin finite element method, which is carried out jointly with H. Atkins (NASA Langley), is in the phase of analyzing the effect of limiters and artificial viscosities for very high order (order from 4 to 10) versions of the scheme. These schemes are L^2 stable for nonlinear scalar problems even without such limiters or artificial viscosities, however mild limiters or viscosities will render the scheme more robust. Jointly with G. Erlebacher and M.Y. Hussaini, we are continuing our investigation of shock longitude vortex interaction problem. It is found out that steady state may not be reached, hence the result may depend on the initial conditions.

Research will be continued for high order methods in finite difference, finite elements and spectral schemes.

DAVID SIDILKOVER

New discretization schemes and fast solvers for steady-state inviscid flow equations

One of the popular approaches towards the construction of discrete schemes for incompressible flow computations is based on the so-called Pressure Poisson Equation (PPE) formulation of the flow equations. Such a formulation (unlike the standard one) when discretized on a non-staggered grid does not admit any unstable modes in pressure. It also allows to construct a very simple and efficient multigrid solver. The drawback, however, is that the additional boundary conditions for pressure need to be derived and properly treated within the relaxation process. The goal of this work is to construct efficient multigrid solvers based on

- PPE approach for the inviscid incompressible case with simplified treatment of the pressure boundary conditions;
- extension of this approach to the compressible (subsonic) case.

A scheme of the fluctuation-splitting type was constructed for the incompressible case using a PPE-like approach. Such a scheme implies the proper construction and treatment of the pressure boundary conditions. The relaxation becomes, therefore, remarkably simple. One can obtain a multigrid efficiency identical to that for the Poisson equation, provided the relaxation was performed in the flow direction. This approach extends to the compressible case in a quite straightforward way.

The plans for the near future include generalizing the developed techniques for the viscous and time-dependent cases both concerning the incompressible flow.

Fast potential flow solver

Availability of a fast and accurate solver for Full-Potential equation is not only for being able to compute potential flow efficiently, but to construct a fast solver for the Euler equations. This is because the Full-Potential operator represents the non-advection factor of the Euler system. The main obstacles in constructing an efficient potential flow solver are the following:

- changing type of the equation (elliptic in the subsonic regime and hyperbolic in the supersonic regime);
- anisotropy in the transonic regime;
- difficulty of combining second order accuracy with non-oscillatory property in the transonic and supersonic regimes.

This work is being done in collaboration with S. Ta'asan (Carnegie-Mellon University).

We start from the original Murmann-Cole scheme, which is second order accurate in the subsonic regime and first order accurate in the supersonic regime. Second order accuracy for the supersonic case is achieved by incorporating the multidimensional corrections/limiters. Such non-linear correction does not impede the stability/smoothing properties of the relaxation. The optimal multigrid performance for the entire range of the flow regimes can be achieved. This requires the use of semi-coarsening technique for the transonic case.

The future plans include further generalization of the algorithm for arbitrary flow direction. The next step will be the incorporation of the algorithm within a solver for the Euler equations.

RALPH SMITH

Numerical approximation of thin shell dynamics

In a large number of structural and structural acoustic applications, the dynamics of the underlying structure can be modeled by thin shell equations. Before simulations, parameter estimation, or controllers can be implemented, these equations must be discretized in a manner that is accurate, efficient and preserves the asymptotic properties of the system. During the time period covered by this report, we have investigated the development of a spline-based Galerkin method for approximating thin shell dynamics. This research was done in collaboration with R. Del Rosario.

A cubic spline/Fourier basis provided sufficient accuracy for adequately resolving shell dynamics while remaining flexible in applications. For example, the basis is easily adapted to the various boundary conditions which arise in experimental setups. Moreover, the presence and contributions from actuators such as piezoceramic patches are easily incorporated in the physical parameters for the system. Hence the method can be used to discretize smart material systems in a variety of experimental conditions.

The approximation method will next be combined with finite dimensional control theory to develop PDE-based controllers for shells and structural acoustic systems involving shells. Once the numerical development of these controllers is completed, issues regarding experimental implementation will be considered.

Implementation of PDE-based controllers for structural acoustic systems

Recent investigations have demonstrated that PDE-based controllers employing piezoceramic actuators can be experimentally implemented in structural applications. Numerical studies have also illustrated that through careful modeling and utilization of the coupling between the structural vibrations and adjacent acoustic fields, PDE-based techniques can be used to reduce structure-borne noise in structural acoustic systems. Currently, issues concerning the experimental implementation of these methods in structural acoustic systems is under investigation. This research was done in collaboration with H.T. Banks.

In collaboration with M. Demetriou (Center for Research in Scientific Computation), the effects of modeling and measurement uncertainties are being numerically tested. Numerical techniques facilitating real-time integration of the state estimator and tracking equations are also under development. To attain real-time implementation, it is also necessary to optimize the hardware and software used in actual experiments. This involves the use of multiprocessor digital signal processing (DSP) boards with *C* and assembler code used for interfacing and actual control computations. The development of this code is being performed by R. Del Rosario (North Carolina State University) and D. Brown (Acoustics Division, LaRC) with R. Silcox (Acoustics Division, LaRC) collaborating on structural and acoustical aspects concerning the experiments.

Upon completion of robustness studies and development of experimental control software, we will begin experiments with a structural acoustic system consisting of a hardwalled chamber with a vibrating plate at one end. These experiments will be performed in the Acoustics Division, LaRC.

SHLOMO TA'ASAN

Canonical-auxiliary variables formulation for inviscid flows

The motivation of this work was to extend previous results concerning fast solvers for inviscid flows, to non-staggered grids. Textbook multigrid convergence is aimed in all range of Mach numbers.

The approach is to introduce auxiliary variables both in two and three dimensions such that velocity components are derived from them. The other variables in addition to the auxiliary variables are entropy and total enthalpy. Conservative discretization of the inviscid equations are derived. The scheme is constructed for general unstructured as well as structured meshes where variables are located at node. It employs symmetric stencils which are *h-elliptic* for the elliptic part of the problem, and upwinded only for hyperbolic quantities. Numerical experiments in two dimension with these schemes for compressible and incompressible cases show efficiencies similar to those obtained previously for staggered meshes, i.e., textbook multigrid convergence.

Extension of the ideas to three-dimensional flows, both internal and external is being considered.

Pseudo-time methods for optimization problems

The motivation of this work was to develop optimization techniques for problems arising in aerodynamics. The goal is to solve the optimization problem while the analysis problem is being solved. However, the emphasizes is on methods that do not necessarily use multigrid solvers.

The idea of the new methods is to embed the necessary conditions into a pseudo-time evolution process that can be shown to converge using an energy estimate. The type of embedding used is to

consider the design equation which is defined on the boundary of the shape as an extra boundary condition for the extra unknowns, i.e., the design variables. Thus, at each time step for the state and costate equations, their boundary conditions together with the design equations are being satisfied. Numerical experiments with the methods on a few model problems have shown that the performance of the method is independent of the number of design variables.

Extension of the work to Euler solvers that use canonical variables multigrid solver is being considered.

HILLEL TAL-EZER

Iterative algorithm for general non-symmetric linear systems

As technological developments expand our computational power, we are encouraged to solve very large problems. In particular, it is observed that the solution of linear algebraic systems is a fundamental, and often the most time-consuming, part of many simulation codes. In many such systems, specially those which result from simulating partial differential equations, the matrices are huge and sparse. This means that relatively few entries of the coefficient matrix $\mathbf{A}$ are nonzero. Hence one has to resort to iterative approach in order to take full advantage of the sparseness of the matrix. While direct methods have achieved maturity and can be considered ‘robust’, this is not so for iterative methods. There is no one method which can be considered robust. One of the leading algorithm is GMRES (Generalized Minimum Residuum). While it can have reasonable rate of convergence for many problems, it still suffers from stagnation phenomenon in many cases.

A research was conducted to overcome this lack of robustness. One can show that there is a domain in the complex plane, larger then the spectrum, such that GMRES stagnates if and only if, zero is in this domain. Based on this knowledge, we have developed an algorithm which combines GMRES strategy with Complex Space Approximation algorithm (a generalization of Chebyshev algorithm to any domain in the complex plane) . The algorithm which results is much more efficient and robust then GMRES. It reduces the stagnation phenomenon significantly. Numerical test on real-life problems were taken and the results verified the improved robustness.

An additional efficiency can be gained by optimizing the parameters which control the switch from one approach to the other. We intend to do it in the on-going research.

CHRISTOPHER TAM

A finite difference scheme for computational aeroacoustics problems with disparate length and time scales

Many aeroacoustics and unsteady fluid dynamics problems involve disparate length and time scales. We wish to investigate the possibility of developing an accurate and efficient finite difference algorithm for the computation and simulation of this class of problems.

We adopt a multi-domain strategy. That is, grids of different sizes are used in different regions of the physical domain according to the local resolution requirement. A high-order central difference scheme (we prefer the Dispersion-Relation-Preserving scheme) is used in each of the regions except in the buffer zone where there is an abrupt change in grid size. Optimal finite difference stencils

in the buffer zone are developed. The coefficients of the stencil are optimized in the wavenumber space.

It is recognized that spurious numerical waves are inevitably generated as the physical waves pass through the buffer zone. A way to suppress the generation of spurious numerical waves is to add artificial damping in the finite difference scheme. We plan to design special damping stencils for the buffer zone. This aspect of the work will be continued in the coming months.

ELI TURKEL

Preconditioning

Together with Veer Vatsa of NASA Langley, we are testing preconditioning for three dimensional flows with complicated geometries. It is well known that most codes have great difficulties solving problems when the Mach number is too low. These difficulties involve both very slow convergence rates to a steady state and also accuracy difficulties even once a steady state is achieved. Though the flow is almost incompressible there are numerous instances that one cannot use an incompressible code e.g. transonic flow in a small portion of the domain. Preconditioning is a technique for overcoming these deficiencies. This is based on changing the eigenvalues of the inviscid system so as to more equalize them for low speed flow. At the same time the artificial viscosity, or Roe matrix, is modified. These two changes improve both the convergence rates and the accuracy.

We are calculating the inviscid flux terms as in the standard TLNS3d approach. This is then multiplied by a matrix which simultaneously preconditions the residual and converts it to (p,u,v,w,T) variables. We then add the artificial dissipation and calculate the primitive variables at the next stage of the Runge-Kutta method. Finally the conserved quantities are calculated. Thus the preconditioned quantities are used for both residual smoothing and multigrid transfers. We have much improved results for both inviscid and viscous three dimensional flow about an ONERA wing at an inflow Mach number of 0.01. We have also applied this preconditioner to a multi-element two dimensional viscous case with an inflow Mach of 0.2 with equally dramatic speed-ups in the convergence rate.

We are developing a matrix valued artificial viscosity for the preconditioned equations. We will also extend the applications to some interior flow situations.

Cusp & Slip schemes

The second project, together with R.C. Swanson of NASA Langley, is a study of the CUSP scheme devised by Antony Jameson. This scheme uses a splitting of the convective and pressure terms and gives an alternative artificial viscosity to the matrix viscosity previously developed by Swanson and E. Turkel.

We have programmed up the HCUSP scheme and a preliminary version of SLIP. This is based on the published papers of Jameson and coworkers. Some preliminary runs show that the CUSP scheme gives a sharper shock (one point in the shock rather than two) but that the lift and drag are not as good as with the matrix viscosity. However, the new scheme does seem to give improved solutions at the trailing edge for viscous flow.

We intend to test these two schemes on many more difficult cases to get a better unbiased feeling of the advantages and disadvantages of each method. This will also enable us to develop a new method possessing the advantages of the current algorithms.

High aspect ratios

The third project is in its initial stages. One of the major drawbacks of current CFD methods for steady state aerodynamics is their slow convergence rates. Using a multigrid acceleration technique one requires about 2000 explicit sweeps through the mesh to reduce the residual by about four orders of magnitude for a typical viscous calculation. Implicit methods are slightly faster but not by very much. One of the main drawbacks seems to be the very high aspect ratios required for high Reynolds number flow. This high aspect ratio implies that a scheme that is efficient in one direction is not efficient in the other direction. Hence, smoothing rates for the multigrid acceleration are close to one.

We propose to use an implicit/explicit method that automatically uses different schemes in the different directions. As a start we are analyzing the use of an explicit/implicit residual smoothing algorithm with coefficients that depend on the aspect ratio. All quantities including the CFL and Runge-Kutta coefficients will ultimately depend on the aspect ratio of each cell.

This new method will first be tested on a boundary layer flow with a Cartesian mesh and a fixed aspect ratio. Later work will extend this to general non-orthogonal meshes and eventually to three dimensions.

BRAM VAN LEER

Local preconditioning of the Euler and Navier-Stokes equations

Local preconditioning of PDE systems such as the Euler and Navier-Stokes equations has a number of numerical benefits arising from the equalization of the different convective and diffusive time scales achieved by the preconditioning. A major problem to be resolved is how to make the symmetric Euler preconditioner ($\text{Re}_\Delta = \infty$), previously derived by Van Leer et al., effective for any combination of Reynolds number and Mach number.

We have previously considered a preconditioning matrix that is the sum of the Euler preconditioning, suited for the PDE system, and the Jacobi block generated by upwind differencing of the viscous and conductive terms, which are proportional to Re_Δ^{-1} . This hybrid analytical/numerical approach is unsatisfactory for low Re_Δ . Instead we used the analysis of Merkle, Venkateswaran et al., in which only one entry of their Euler preconditioning is made Re_Δ -dependent. A dispersion analysis for a simplified NS-system uncovers what the proper limits are for $\text{Re}_\Delta \rightarrow 0$, $M/\text{Re}_\Delta \rightarrow 0$, and $\text{Re}_\Delta \rightarrow 0$, $M/\text{Re}_\Delta \geq O(1)$.

The correct form of the modification for the Van Leer preconditioning has not yet been obtained, but a preliminary form may be tested in the near future.

V. VENKATAKRISHNAN

Solution techniques for unsteady flows on unstructured grids

The objective of this work is to develop efficient unsteady flow solvers to be able to handle flows past complex configurations possibly in relative motion.

The implicit method that has been selected for computing unsteady flows is a dual time-stepping method. The outer time step is the physical time step which is solely determined by the flow physics and not by stability considerations. The inner time step is a pseudo time step, where accuracy in time is not an issue, thus permitting the use of conventional acceleration techniques such as local time stepping, residual averaging and multigrid. The implicit method has been validated by computing a variety of unsteady flows. For bodies in relative motion, grid generation is an important issue. Regeneration of the grid is unattractive and conventional means of deforming the grids using spring and other analogies, invariably fail. In our approach, we augment the spring analogy with a reconnection procedure, so that the grid remains valid even for large displacements of the bodies. Also, when computing compressible flows with shocks, conservation in time is an important consideration. Usual methods of satisfying this property are diffusive and compromise the second order accuracy of the scheme. We have derived conservative, linearity-preserving interpolation formulas that also do not introduce new extrema. Another aspect that has been investigated is the so-called Geometric Conservation Law, which states that simply moving the grid through a uniform field should not change the solution. A formulation that preserves uniform field for arbitrary motion of the grid has been derived for the implicit scheme that makes use of three time levels.

This work has been done in collaboration with D.J. Mavriplis.

A new effort has been initiated in the area of higher order accurate schemes on unstructured grids. Even though these methods have been investigated by researchers in the past, they are seldom used in practice. A number of ideas from the finite volume and finite element literature are being pursued. The objective of this research is to fully understand the capabilities and limitations of the various approaches in one and multiple dimensions for test problems and to extend the methodology to solve the Reynolds averaged Navier-Stokes equations with field equation turbulence models.

HONG ZHANG

Multigrid waveform relaxation for hyperbolic equations

The multigrid waveform relaxation algorithm is an efficient time parallel solver for certain type of time dependent PDE's. During my two year visit at ICASE (1992-94), in collaboration with S. Ta'asan, we have studied and implemented the algorithm for parabolic equations. It has been found that the multigrid performance of the waveform relaxation for a parabolic equation is similar to that of static iteration for the related steady-state equation. However, the properties of the multigrid waveform relaxation method for hyperbolic problems are relatively unknown. We have done case studies on the convergence factor of the multigrid waveform relaxation method for problems which are not elliptic, or in which the elliptic principal part is small. Many problems in fluid dynamics, and in other fields, are of this type.

We have been investigating the relationship between the multigrid waveform relaxation method for time-dependent hyperbolic equations and the multigrid method for the corresponding steady-state problems, with focus on their quantitative convergence comparison. The Fourier method is a powerful tool for convergence analysis of numerical schemes for hyperbolic problems. Fourier-Laplace analysis, i.e. Fourier analysis in space and Laplace transform in time, has been performed in two case studies. Interesting phenomena have been observed. In particular, it has been found that, the multigrid waveform relaxation could diverge for a hyperbolic equation while its steady-state analogue worked well on the associated steady-state problem. The experimental results have confirmed our findings.

Future plans include the investigation of other acceleration techniques to the waveform relaxation method and the application of the method to real world problems.

FLUID MECHANICS

FRANCOISE BATAILLE

Energy transfer in compressible turbulence

This study investigates energy transfer in compressible turbulence. We extend a methodology developed originally for incompressible turbulence and use data from numerical simulations of weakly compressible turbulence based on the Eddy-Damped-Quasi-Normal-Markovian (EDQNM) closure. This work was done in collaboration with Y. Zhou.

In order to analyze the effects of the compressibility, the velocity field is decomposed into solenoidal and compressible components. Using an EDQNM model, it is then possible to obtain energy transfer equations in the case of weakly compressible turbulence. We find that the solenoidal triadic energy transfer is not affected by the compressible component. A study of the compressible triadic energy transfer shows that the compressible mode receives energy from the solenoidal part and that the energy is added and removed locally.

In the future, a more accurate study of compressible triadic energy transfer will be done by decomposing all the terms which appear in the compressible transfer.

Numerical simulation of compressible turbulence

Using the EDQNM closure, simulations of forced isotropic turbulence lead to the conclusion that the irrotational velocity spectrum scales as $k^{-5/3}$ in the inertial range for short times and has a long time asymptotic state which scales as $k^{-11/3}$. The aim of the study was to find out whether this behavior could be reproduced through a large-eddy simulation of decaying isotropic turbulence. This work was done in collaboration with G. Erlebacher and M.Y. Hussaini.

We tested several initial conditions. Among these, we considered both analytical and experimental initial spectra. The effects of Reynolds number and degree of isentropy were considered. Results show quite convincingly that the $k^{-5/3}$ and $k^{-11/3}$ behavior could be recovered, even on grids as coarse as 64^3 . Although the predicted spectral powers were sometimes difficult to obtain (for example at high Reynolds number), they appear clearly in most of the simulations. Note that EDQNM predicts that the $k^{-11/3}$ spectrum takes longer to established itself the higher the Reynolds number. Both the Smagorinsky and the dynamic subgrid scale models led to similar results. Therefore, it does not appear that a more complex subgrid-scale model is required for the calculation of spectral slopes in isotropic turbulence.

In the future, it would be interesting to study the dependence of the compressible spectrum on the turbulent Mach number and to conduct simulations of forced isotropic turbulence.

ALVIN BAYLISS

Jet noise/structure/flow field interaction at transonic and low supersonic speeds

The objective of this work is to study numerically the interaction between acoustic disturbances in a jet and an array of flexible aircraft-type panels. Sound from jet engines is a major source of the loading on aircraft panels. The vibration of these panels can contribute to their structural fatigue and lead to increased interior noise levels. While the panel response can be modeled by computer for any prior specification of the sources, an accurate and self-consistent simulation of panel response requires computation of the acoustic response of the jet in a manner that is fully coupled to the panel source. We have developed a computer code which accomplishes these objectives subject to the restriction of two dimensionality. This research was conducted in collaboration with L. Maestrello of NASA and C. Fenno who is an NRC postdoc.

During the past year we have concentrated on (i) the incorporation of forward motion into our model thus simulating an aircraft in flight and (ii) the effect of transonic and low supersonic jet speeds on panel response and radiation. We showed that the effect of forward motion is stabilizing, in that it reduces the level of instabilities in the jet. Forward motion leads to a reduction in sound level downstream of the jet and an amplification of sound upstream. There is a similar effect on panel response and radiation; thus the effect of forward motion on panel response is heavily dependent on the location of the panel relative to the jet exit. In our consideration of transonic flows, we find that for long times the computed jet response peaks within the frequency range observed in experiments. There is also a marked increase in panel response in this regime.

In future work we will extend our calculations to the supersonic regime. We will also determine the effect of nozzle geometry on both jet and panel response. We also plan to account for boundary layers on the panels. We have developed a cylindrical version of our code and will extend our calculations to account for axisymmetric jets.

STANLEY A. BERGER

Turbulence/free-surface interaction

There are important technological problems involving the interaction of turbulence and free surfaces. Little is known about the physics and the appropriate modeling of this interaction. There has been some experimental work and some DNS simulations, but these are still very much in the early stages of investigation. The objective of our work is to find a computationally practical turbulence modeling approach which captures the important physics, and yields the required physical quantities of interest.

Since DNS is impractical for these inherently large Reynolds number problems, we have primarily concentrated on LES and unsteady RANS simulations as the most likely candidates to model turbulence/free-surface interactions. Our first efforts have been directed at the use of RANS methods, using state of the art turbulence closures, particularly full Reynolds stress models as well as simpler explicit algebraic stress models. To do this boundary conditions for turbulence quantities at the free surface must be determined. We have begun to identify and pull together the experimental and DNS data necessary to do this.

Having identified the appropriate boundary conditions at the free surface we plan to carry out the RANS simulations, both steady and unsteady, described above. A number of generic problems will be analyzed, such as a turbulent jet discharged below and parallel to a free surface. We also plan to study these problems using VLES, Very Large-Eddy Simulations, as an alternative to LES.

JEAN-PIERRE BERTOGLIO

Comparison between a two-point closure theory and L.E.S. data for compressible isotropic turbulence

One of the results of EDQNM (two-point closure theory) for weakly compressible turbulence is the prediction of a $k^{-11/3}$ spectrum for the purely compressible modes at low Mach number. Large-Eddy Simulations are being performed both at ICASE and at Ecole Centrale de Lyon (LMFA) to validate this prediction. We tried to understand why this result was confirmed by the ICASE L.E.S. data obtained in the case of decaying isotropic turbulence, (and using a Smagorinsky subgrid model), and not by the French L.E.S. performed in the case of statistically stationary (forced) turbulence (using an extended Chollet Lesieur subgrid model).

We therefore began to implement the forcing technique used in Lyon in the ICASE code. We also ran the LMFA code with a Reynolds number corresponding to one of the ICASE simulations. Results have shown that the $k^{-11/3}$ can be obtained also in the case of forced turbulence.

We plan to make more refined and quantitative comparisons and investigate the influence of the Mach number. This work was done with G. Erlebacher, F. Bataille, and L. Shao (in Lyon, by e-mail).

TIMOTHY T. CLARK

Spectral turbulence models and engineering closures

A simple spectral model for inhomogeneous anisotropic turbulence has recently been proposed by Besnard, Harlow, Rauenzahn and Zemach. This model uses a simple advection/diffusion approximation to describe transfer of turbulence quantities in k -space, and thus is referred to as the Local Wave Number (LWN) model. More recently, Clark & Zemach have presented successful comparisons of LWN predictions with experiments and with theoretical results. Additional tests, refinements and extensions are necessary to: (1) improve the current model, and (2) provide a description of a broader range of problems of importance to the engineering community.

The derivation of the two-point correlation equations for the passive scalar problem in the general case of inhomogeneous turbulence has been pursued. This provides the starting point for the derivation of an "LWN-like" closure for passive scalars. The resulting model may be anticipated to possess a wider range of validity than current engineering models in flows with widely divergent time scales and length scales, or turbulence subjected to rapid transients. In addition, some useful tests of spectral models were identified during discussions with staff members at ICASE (in particular, J. Ristorcelli and R. Rubinstein). The central "theme" of these tests is to understand how turbulence "decorrelates" in time as a function of length-scale (or wavenumber) while undergoing rapid transients, e.g., strong homogeneous shears and/or strains.

We plan to complete the extension of LWN to include the behavior of passive scalars, to test the LWN in a varied regime of combined mean-flow shears and strains, and to pursue a fully three-dimensional Fourier space description of a turbulence field undergoing transients that is consistent with rapid distortion theory.

WILLIAM O. CRIMINALE

Perturbation vortex dynamics

New closed term solutions to the Navier-Stokes are derived. General three-dimensional perturbations are introduced into a fully three-dimensional vortex that is under strain. The complete perturbation problem is solved in closed form even when very general arbitrary initial data are given.

We find that it is the radial variation of the velocity disturbance that is the most important factor influencing the qualitative behavior of the solutions. More interesting is the finding that transient growth of the velocity amplitude is directly attributable to the localness of the initial vorticity. This work was done in collaboration with T.L. Jackson and D.G. Lasseigne.

This work is unique and has potential for extensions to more complicated incompressible vortices as well as vortices in a compressible fluid. It marks one of the first times that a stability analysis is possible for flows of complicated geometry and is important in both aeronautics and geophysical fluid dynamics.

The laminar boundary layer

Solutions to the time-dependent linearized Navier-Stokes equations are solved without assuming spatial separability (as is usually done). Instead, the linear equations are integrated in time with various initial expansions for the spatial dependence taken in order to meet the boundary conditions. Classical results known from traditional stability theory can be reproduced along with the (important) entire early transient period.

We find that any resulting flow in the disturbance field depends upon the particular choice of initial conditions and whether or not the freestream boundary condition is one that decays or is merely finite. The finite condition leads to more energetic excitation within the layer (to the order of 10% or more for the cases considered to date). The method will be extended to include the more general problem of receptivity or the boundary layer interacting with the freestream (turbulence, for example). This work was done in collaboration with T.L. Jackson and D.G. Lasseigne.

We further expect to link this effort with a full numerical compressible Navier-Stokes code. This approach can be adapted to fully explore the possibility of flow control.

AYODEJI O. DEMUREN

Higher-order accurate compact schemes for incompressible flow simulation

It is generally accepted that higher-order accurate methods are required for direct simulation of turbulent flows, but large-eddy simulations are often performed with second-order methods. However, on practical computational grids, these methods suffer from dissipation and dispersion

errors which corrupt the flow physics. Compact schemes have been shown to be highly accurate in computations of compressible flows in simple geometries. The solution of the continuity equation to obtain a divergence-free field presents additional difficulty in incompressible flows, since there is no suitable evolution equation.

In collaboration with R. Wilson and M. Carpenter, fourth- and sixth- order accurate methods are developed for simulation of incompressible flows based on corresponding compact finite-difference formulations. To satisfy the divergence-free condition for the velocity field, a Poisson equation is derived for pressure which must also be solved by the same compact scheme for consistency. Furthermore, to deal with complex computational domains, grid transformations are required, for which the metric terms should also be computed with the corresponding compact scheme. The accuracy of these methods has been demonstrated with several benchmark problems. The fourth-order method was found to be considerably more accurate than a comparable ENO scheme.

Work is now progressing on the generalization to curvilinear grids, and the simulation of complex turbulent jets.

GORDON ERLEBACHER

High mach number shock-vortex interactions

Fundamental understanding of shock-turbulence interaction, both from the point of view of acoustics, and that of turbulence modeling remains a primary research target. It is known from large scale Direct Numerical Simulations (DNS) of the compressible Navier-Stokes equations that shocks amplify the vortical component of turbulence, and generate acoustic pressure waves. However, the conditions are under which linear theory breaks down are not clear. A quantitative understanding of these conditions, along with input from current 3-D simulations will permit better turbulence models to be constructed.

Using a 6th order compact scheme in space, and a 4th order time advancement scheme, we have applied our shock-fitted code to study the interaction of weak and strong disturbances with a planar shock. These disturbances take the form of compact vortices, which amplify as they cross the shock, and contract in the direction normal to the shock. Budgets of vorticity and dilatation indicate that, keeping the vortex circulation constant, nonlinearities become more important as the shock Mach number increases. We have confirmed this result by performing a large Mach number expansion of the linearized Rankine-Hugoniot conditions. This in turn leads to the conclusion that the threshold between linear and nonlinear regimes is delineated by the product of shock Mach number and vortex circulation, thus confirming the numerical results.

To investigate detonation-turbulence and detonation-vortex interactions, the code will be modified to include reaction via a simple one-step heat release mechanism with a finite-length reaction zone.

SHARATH S. GIRIMAJI

Fully-explicit, self-consistent algebraic Reynolds stress turbulence model

The current explicit Reynolds stress model in the literature is poorly behaved in an important parameter range of strain-rate and enstrophy. For the example, in the high-lift air foil calculations

ad hoc modifications are sometimes necessary to achieve reasonable results. The objective of this project is to derive a fully explicit algebraic Reynolds stress model which is self-consistent and numerically well behaved even in complex flow situations.

By treating the production of turbulent kinetic energy explicitly, a preliminary version of the model has been derived. The model is a function of the turbulence time scale and the mean strain and rotation rates only.

For the future, further refinement and extensive testing of the model are planned. Certain important uniqueness issues of the model must be addressed.

Algebraic Reynolds stress model for curved flows

Most flows of engineering importance are characterized by curved mean streamlines. The current algebraic stress model violates the Galilean invariance requirement for these flows necessitating a new modeling approach.

Work is underway to derive an algebraic Reynolds stress model that is both sensitive to streamline curvature and Galilean invariant by invoking the weak equilibrium assumption in an objective coordinate system. The initial indications are promising.

It is imperative that the model be explicit in nature, requiring no iterative procedure to solve for the Reynolds stresses. Once the model derivation is complete, extensive tests are needed to evaluate its capabilities.

Direct numerical simulations of scalar mixing and utilization of data to validate a LES scalar dissipation model

Large eddy simulation (LES) is considered by many as the future tool for computing complex turbulent reacting flows. However, several important advances in the subgrid scale models must be made before LES can be considered a viable tool.

A challenging project to derive a model for large eddy scalar dissipation is still in progress. Models have been developed using Renormalization-Group type approach and with guidance from direct numerical simulation data. These models are being continually refined and fine-tuned.

A priori and *a posteriori* checks of the model need to be performed in the future.

CHESTER E. GROSCH

Mixing enhancement in a hot, supersonic jet

Experimental observations show that the presence of small “tabs” on the edge of a hot, compressible jet exiting into a slower moving, colder ambient flow can increase the rate of spreading of the jet. This suggests that the rate of mixing of the jet and the ambient fluid is also increased. We wish to simulate this effect in order to (1) elucidate the physical mechanism responsible for the increased spreading rate and (2) perform a parameter study to find ways to further increase the effect.

I have carried out a set of calculations, in conjunction with T.L. Jackson, using a compressible Navier-Stokes code. We have simulated the flow without the “tabs”, obtaining very good agreement with experimental measurements of the velocity. Simulations with modeled “tabs” were also carried out. In these calculations the “tabs” were modeled by pairs of counter-rotating vortices. The results

of these calculations indeed show that the presence of the “tabs” increases the spreading rate of the jet. The basic physical mechanism responsible for the enhanced spreading rate was found. A series of preliminary parametric studies was carried out with the results showing the dependence of spreading rate on the parameters of the vortices.

Next, we plan to obtain the experimental data gathered with “tabs” present and compare these with the results of the computations. Other cases, for which experimental data are available, will be simulated both with and without “tabs”. In addition, the use of oscillating “tabs” will be simulated.

ALI H. HADID

Assessment of Gatski-Speziale explicit algebraic stress model in turbulent separated flows

Turbulent flows of practical engineering interest such as those found in turbomachinery and combustion devices are in general very complex and an adequate description by the commonly used two-equation eddy viscosity models is often difficult to achieve. Second order closures based on the solution of extra transport equations for the individual stress components are, on the other hand, expensive. A recently proposed explicit algebraic stress equation for the Reynolds stress tensor by Gatski and Speziale extends the range of applicability of the two-equation eddy viscosity models by accounting for rotational and irrotational strains and of stress anisotropy. Moreover, the explicit nature of the model helps to reduce numerical problems associated with inverting a stress matrix at each step of the calculation as required in the traditional implicit models.

The explicit algebraic model is implemented in a finite-volume method that solves the Navier-Stokes equations on non-orthogonal grids with a collocated grid arrangement. The model is applied within the context of a $k-\varepsilon$ two-equation model to separated two-dimensional backward facing step flow. Preliminary results show improved predictions over the standard $k-\varepsilon$ model when compared with the data of Driver and Seegmiller.

It is planned to compare the performance of the explicit algebraic stress model with the more elaborate full Reynolds stress model of Speziale, Sarkar and Gatski. The model will also be used to analyze flows of engineering interest where the effects of streamline curvature, rotational strains and secondary flows due to turbulence and anisotropy can be accounted for. These effects are important in swirling flows and combustion devices for example, and in complex 3D flows in turbomachinery components such as inducers and impellers.

PHILIP HALL

Phase equations and shear flow transition

The evolution of large amplitude wavesystems in shear flows must be determined if the gradual onset of transition is to be understood. In particular the stability of different nonlinear equilibrium states needs to be understood.

The phase equations for two and three-dimensional Tollmien-Schlichting wave systems in shear flows have been obtained. The approach yields a rational way for the determination of the wavenumber evolution of a wavesystem in the nonlinear regime. A particular case of interest is the one where

the wavenumber is almost constant. Here the phase equation approach yields an evolution equation for a wavenumber perturbation. We have shown that the generic wavenumber evolution equation is Burgers equation. Results have now been obtained for channel flows and boundary layer flows in both the supersonic and subsonic regimes.

Future work will be concerned with the hypersonic limit and the effect of control methods on the evolution process. A numerical investigation of the evolution equations in the general case will be carried out.

Non-equilibrium critical-layer theory

The nonlinear stability problem for inviscid Görtler vortices in a slightly swept wing flow is a fundamental problem in the transition process in three-dimensional flows over wings with regions of concave curvature. This study aims to shed light on that process. This research was conducted in collaboration with N. Blackaby and A. Dando.

The Görtler modes we consider are initially fast growing and we assume, like similar studies, that boundary-layer spreading results in them evolving in a linear fashion until they reach a stage where their amplitudes are large enough and their growth rates have diminished sufficiently so that amplitude equations can be derived using weakly nonlinear and non-equilibrium critical-layer theories. We find that the amplitude equation can take three forms. These are a cubic due to viscous effects, a cubic which corresponds to the novel mechanism investigated in previous papers and a quintic. We concentrated on the two cubics. We find that the consideration of a spatial, rather than a temporal, evolution problem causes a number of significant changes to the evolution equations.

Future developments will concern the evolution of the disturbances into more nonlinear states. The possible interaction of this type of disturbance with TS waves or other inviscid modes will be investigated.

Wavy vortex structures at high amplitudes

The large amplitude structures which exist in highly curved flows in channels or between concentric cylinders are not yet fully understood. Previous theoretical work has been restricted to small amplitudes whereas full scale numerical simulations are costly. The aim of this project is to derive an alternative theoretical approach valid at larger amplitudes. This research was conducted in collaboration with A. Dando and D. Papageorgiou.

We have derived a new evolution equation for very large amplitude disturbances in curved flows. The nonlinear term is quite distinct from that of small amplitude theory.

We hope that the equation will reveal information about the interaction of different wavy vortex modes in curved flows. The numerical solution of the evolution equation is underway. A version of the equation relevant to modulations in the spanwise direction will be derived.

KEMAL HANJALIC

Low-Reynolds number and wall-proximity effects in second-moment turbulence closures

Modification of the second-moment closure models to account for viscous and wall-proximity effect in terms of invariant parameters has been pursued aimed at developing a new model based on

a sounder physical basis and a more rigorous derivation. The model should allow the integration to the wall (avoidance of wall functions) and reproduce relaminarization and some forms of laminar-to-turbulent transition (bypass transition and proper amplification of inactive background turbulence e.g., in oscillating and pulsatile flows at transitional Reynolds numbers).

Attention is focused on the dissipation equations and its components ε_{ij} . The current practice in modeling the low-order terms has been reexamined and a new model formulation has been sought which will enable full elimination of wall-topography related parameters (wall distance, unit normal vectors) and better satisfy the turbulence asymptotic and limiting states (infinite and vanishing turbulence Reynolds numbers, two-component limit etc.).

Explicit algebraic modeling of turbulent buoyancy driven flows and heat transfer

A full second moment closure model for turbulent heat transfer can be derived and closed by applying analog reasoning as in modeling the stress transport equations in isothermal flows. Such a model contains a large number of differential transport equations and is burdened by large uncertainty in modeling various terms, particularly in cases with strong thermal buoyancy. The need to solve the equations up to the wall with a fine grid resolution in the near-wall regions with very steep variation of all flow properties aggravates further the application of the full differential model in complex flows. A promising route to overcome the problem in the near future is the use of an algebraic stress/flux model which solves the differential transport equations only for scalar properties: turbulence kinetic energy, temperature variance and their dissipation rates. This approach has been shown to reproduce well a number of buoyancy driven flows in different geometries and with various boundary conditions.

Current practice employs either the implicit algebraic formulation of turbulent heat flux based on Rodi's approach to the truncation of the evolution equations, or the explicit formulation by full neglect of the transport terms. This work uses the vector representation theorem to formulate an irreducible integrity basis which should yield an explicit algebraic model while retaining Rodi's treatment of the evolution transport terms. This work has been done in collaboration with S. Girimaji.

MICHAEL S. HOWE

Sound generated by a vortex interacting with the edge of an elastic plate

A variety of noise sources contribute to aircraft interior (cabin) noise. The component of this noise attributable to the high speed turbulent flow over the fuselage is believed to be important for a jet transport in steady cruise. Numerical schemes for its prediction must take proper account not only of sound waves produced by the fluid-structure interaction, but also of structural vibrations generated by the flow that can subsequently generate sound by their interactions with structural inhomogeneities. Such predictions must ultimately be validated by comparison with experiment, but it is also useful to have available a collection of benchmark analytic solutions for comparison.

A canonical fluid-structure-acoustic interaction is being studied. A line vortex is located parallel to the edge of a semi-infinite elastic plate in fluid at rest at infinity. The vortex moves by a self-induction along a trajectory that takes it around the edge of the plate; sound and structural vibrations are generated. The generated sound is known for a rigid plate, and is produced during

the short interval when the vortex passes around the edge. Novel features arise when the plate is elastic. Far from the edge the vortex translates at a constant speed V , say. Its arrival at the edge is preceded by bending wave “forerunners” which are excited in the plate at that frequency f at which the flexural wave phase velocity is just equal to V . These waves have *group velocity* equal to $2V$, and extend over a length of the plate ahead of the vortex determined by the structural damping. In this case, an important additional component of the acoustic radiation must be attributed to the interaction of this forerunner with the edge, and the sound should be predominantly of frequency f . The amplitude of this radiation must increase progressively as the vortex approaches the edge, where it may be expected to be comparable to that produced by motion of the vortex around the edge. Since there is little flexural wave energy in the wake of the vortex, we expect the flexural-wave induced sound to be negligible once the vortex has passed around the edge.

This problem is currently being modeled analytically, by a procedure that makes use of the Rayleigh reciprocal theorem, and will subsequently be treated numerically.

FANG Q. HU

Sound radiation of mixing layers by vortex methods

This study explores the viability of applying vortex simulations for computing sound radiation.

In our approach, the sound radiation from vortex simulations is modeled based on matched asymptotic expansions of the incompressible simulation and compressible far field for small Mach numbers. A model problem of a temporally growing mixing layer has been considered where the acoustic wave equation is solved in the far field. Since the mixing layer is infinitely long, the sound “source” is not compact. The method of matched asymptotic expansions will be employed to find the sound field induced by the motion of vortex blobs. This work is done in collaboration with J. Martin (Christopher Newport University), M.Y. Hussaini (ICASE) and J.C. Hardin (NASA LaRC).

Future work is to extend the analysis and numerical simulation to spatially evolving flows, such as mixing layers and jets. Applications of 3-D vortex methods are also planned.

Absorbing boundary conditions for Euler equations

Recently, a Perfectly Matched Layer (PML) technique has been introduced for absorbing electromagnetic waves. Numerical studies have shown that the PML technique dramatically reduces the reflections of outgoing waves. This work gives a perfectly matched layer for absorbing outgoing waves of the linearized Euler equations.

It is well-known that linearized Euler equations support acoustic waves, which travel at the speed of sound relative to the mean flow, and vorticity and entropy waves, which travel with the mean flow. PML equations for absorbing these linear waves are defined. It is shown that the theoretical reflection coefficient is zero at an artificial boundary, independent of the wave frequency and angle of incidence. This has been verified by numerical examples.

Extensions to nonlinear equations as well as Navier-Stokes equations are being considered as future work. Extension to 3-D calculations will also be carried out.

THOMAS L. JACKSON

Algebraic instabilities in shear flows

Algebraic instabilities arise when some initial disturbances, owing their presence to a finite level of noise present in any flow, grow sufficiently to trigger nonlinear mechanisms or to provide new basic states for secondary instabilities. These instabilities are distinguished from exponential instabilities, where infinitesimal disturbances always grow exponentially in time. The presence of algebraic instabilities may lead to the so-called “bypass mechanisms”. Work is continuing on the evolution of disturbances in viscous shear flows. This work offers a means whereby completely arbitrary initial input can be specified and the resulting temporal behavior, including both early time transients and the long time asymptotics, can be determined. The bases for the analysis are: (a) linearization of the governing equations; (b) Fourier decomposition in the plane and streamwise direction of the flow; and (c) direct numerical integration of the resulting partial differential equations.

The results provide explicitly both the early time transients and the long time asymptotic behavior of any perturbation. With this knowledge it is then possible to devise means for flow control and it is possible to either delay or enhance disturbances as the need may be.

Two classes of problems have previously been investigated: (1) family of free shear flows consisting of the jet, wake, and mixing layer, and (2) viscous channel flows. Current work is focused on the Blasius boundary layer. This method is currently under investigation for the Blasius boundary layer. Future plans will also include viscous pipe flow, as well as the concept of absolute/convective instabilities.

This work is conducted in collaboration with W. Criminale and D.G. Lasseigne.

TSUTOMU KAMBE

Compressive wave phenomena associated with vortices

It is generally well-known that acoustic waves are generated by the collision of vortices, and that a shock wave interacts strongly with a vortex. We have been studying these subjects in recent years. In the shock-vortex interaction, a shock wave is distorted considerably by the vortex flow. In addition, the collision of two shock waves or the intersection of two shock waves are observed in both experiments and computations.

Provided that the shock is weak, the shock distortion would be studied by applying the ray method, which is an extension of geometrical acoustics, i.e., geometrical shock dynamics in the presence of non-uniform flow due to the vortex. In the 2D case of a plane shock wave impinging on a columnar vortex, a system of ordinary differential equations is derived for the position vector and wave vector.

We plan to refine the approach by applying more accurate shock conditions, and also by taking into account the condition of collision or intersection of shock waves.

ASHWANI K. KAPILA

Detonation initiation in reactive media

Detonations in a reactive environment can be generated by a variety of scenarios. Precisely what sequence of events will occur is determined by the initial disturbances in the system.

In earlier work with J.W. Dold (University of Bristol), an asymptotic/numerical approach is used to determine the path to detonation in a system that begins with an initial temperature gradient whose magnitude is of the order of the inverse activation energy of reaction.

The above scenario involves high-speed induction flames that decelerate, produce a shock, and eventually the ZND structure. An alternate series of events occur if the initial gradient is large. That problem is under study in collaboration with J. Quirk (California Institute of Technology, formerly of ICASE).

FRANK P. KOZUSKO

Structure and stability of gases in laminar mixing

The stability characteristics of parallel flow laminar gas mixing was studied using realistic values for the gas transport properties. Results are to be compared with other models using constant or simplified representation of transport properties.

The steady state gas mixture of two parallel flowing gases of different temperatures and velocities was calculated for thirty different combinations of six real gases. The transport properties were dynamically calculated as functions of temperature and gas concentration using various tables or calculated from theory. Neutral phase speeds and growth rates were calculated for all combinations.

This system may be extended to consider reacting flows. This work has been done in collaboration with C. Grosch, T. Jackson and D.G. Lasseigne.

D. GLENN LASSEIGNE

Interaction of oblique shock waves attached to a wedge with three-dimensional freestream disturbances

The response of the flow field behind oblique shock waves to rather general small disturbances upstream of an oblique shock attached to a wedge is being investigated.

The full three-dimensional linearized equations can be solved analytically and the responses to individual vorticity, entropy, and pressure disturbances can be determined. In particular, comparisons can be made to the same system in the absence of the shock in order to quantify the wedge effects. This work is in collaboration with P. Duck and M.Y. Hussaini.

Future work is to test the accuracy of various numerical algorithms in the calculation of oblique shocks. This is possible since the solutions are analytic.

Simulation of laser-initiated oblique detonation waves for supersonic combustion

The use of oblique detonation waves has been proposed for high-speed air-breathing combustion systems. One method of producing such a wave is to turn the supersonic flow using a wedge. A

less intrusive method is to use laser pulses to initiate a series of expanding detonation waves which will approach an oblique detonation in the limit of small time intervals between pulses.

The use of Adaptive Mesh Refinement developed by J. Quirk is proposed to study such a system. The laser pulses will be modeled and the characteristics of the flow will be explored as a function of the strength of the pulses and the time interval between the pulses. Some preliminary calculations have been carried out to adjust the parameters of the AMR routine to this configuration using freestream boundary conditions.

Future work will incorporate shaped walls into the calculations.

ANTHONY LEONARD

New prospects for subgrid-scale modeling

In large-eddy simulations one attempts to follow the evolution of the large scales of a turbulent flow or, in the case of scalar transport, the large scales of the scalar field. This requires modeling the effect of the subgrid scales on the dynamics of the large scales, i.e., a subgrid model. Most efforts to date have relied on Smagorinsky type models that are based on an isotropic diffusion tensor.

Recent efforts have considered the case of scalar transport by a velocity field that is smooth but still produces chaotic advection. In this case one can derive a subgrid model that consists of an anisotropic diffusion tensor.

Present efforts are focused on the possibilities of extending this new model to the fully turbulent regime.

E. DOUGLAS LYNCH

Turbulent combustion in advanced airbreathing propulsion systems

Computational Fluid Dynamics (CFD) has recently been employed as a design tool in the analysis of advanced airbreathing propulsion systems such as ramjets, scramjets and detonation engines. The details and accuracy of analyses of the combustor component in such engines rely heavily on the description of the turbulent combustion process. Previous analyses completed of ramjet and scramjet combustors with normal and axial injection and hydrogen/hydrocarbon fueled pulse detonation engines have usually treated turbulence through equilibrium models not accounting for the effect of turbulence on the reaction rate. However, such methods will not be adequate for many of the types of computations required for ramjet/scramjet missile design – such as transient analyses of ramjet oscillations – where the turbulence is far from equilibrium and fluctuations can have an important impact on ignition and flameholding.

The necessary upgrades in the description of the physics of turbulent combustion have been initiated to analyze such problems computationally. In particular, assumed PDF methods for treating the effect of turbulent fluctuations on the combustion were incorporated within a CFD code previously applied for extensive scramjet and ramjet design computations. The flexibility to incorporate improved physical models including the effect of species fluctuations on the reaction rate and the temperature-species fluctuation coupling effect was also provided.

The next step in developing an improved capability to analyze advanced airbreathing engines will be to validate the assumed PDF model. This will be followed by an application of these improved methods to critical problems in airbreathing propulsion including: 1) Scramjet injector design with large base regions, 2) Ramjet combustion oscillations, 3) The mixing component of the pulse detonation engine cycle. In each of these problems, determining under what conditions ignition will or will not occur is a key design consideration. Finally, additional improvements will be made in the description of the turbulent combustion including extension of the existing capability to analyze a wide range of gaseous fuels to allow for the analysis of storable propellants.

MICHAEL N. MACROSSAN

Particle simulation of near continuum flow; hybrid equilibrium and non-equilibrium scheme

A new high density version of the Direct Simulation Monte Carlo (DSMC) method for high speed low rarefied gas flows was developed by generalizing the Equilibrium Particle Simulation Method (EPSM) to treat multiple species and several degrees of freedom per particle. The EPSM method was developed with a view for use in a hybrid DSMC/EPSM code for situations where a mixture of continuum and rarefied flow conditions can be expected to occur.

An EPSM subroutine has been added to the 3-D DSMC codes of D.Rault of the GDD-Aerothermodynamics branch at NASA LaRC to produce a hybrid DSMC/EPSM code. Initial testing of this hybrid code has been done. It has been found that for high density (collision dominated flow) EPSM is about 3-6 times faster than DSMC with a collision limiter. The overall speed up obtained using the hybrid DSMC/EPSM code depends on the particular problem, that is, on how often the EPSM routines can be invoked rather than the DSMC routines.

The question of quantum energy of vibration in EPSM needs to be addressed. As a first attempt, this will be done by calculating an effective fractional number of degrees of freedom and including a fraction only of the N excited particles in the re-distribution process.

ALEX MAHALOV

Analytical and phenomenological studies of rotating turbulence

The interest in the effects of rotation is reflected in the large body of theoretical, experimental, and numerical work documenting them. As the effects are both multifold and subtle, the development of models which account for the effects of rotation on turbulence requires an understanding of the processes occurring in these flows.

A framework, which combines mathematical analysis, closure theory, and phenomenological treatment, has been developed to study the spectral transfer process and reduction of dimensionality in turbulent flows that are subject to rotation. The approach is based on the Green's method when applied to rotating turbulence. The Eddy-Damped-Quasinormal-Markovian (EDQNM) closure applied to the Poincaré transformed Euler/Navier-Stokes equations leads to expressions for the spectral energy transfer. In particular, a unique triple velocity decorrelation time is derived with an explicit dependence on the rotation rate. This provides an important input for applying the

phenomenological treatment of Zhou. The energy spectrum and the spectral eddy-viscosity have been deduced.

In future work, we plan to compare our model with experimental/numerical data available for turbulent flows subjected to a background rotation. Although the application of the Green's method in complex geometries alters integral convolution kernels in the Poincaré transformed Navier-Stokes equations, the mathematical procedure is still valid provided that explicit asymptotic expressions for the Green's tensor can be obtained. We plan to extend the applicability of our method to certain complex geometries.

JOE MANTHEY

Numerical methods for computational aeroacoustics

Numerical schemes for computational aeroacoustics are studied for application to duct acoustics. Special issues are the implementation of the boundary conditions at the duct walls and outflow boundary conditions. Many existing higher order finite-difference schemes are not time stable and hence are unsuitable for long time integration.

Eigenvalue stability analysis has been performed for high-order explicit as well as compact implicit schemes with the physical boundary conditions applied. It is found that numerical damping is necessary for stability of explicit schemes.

In future work, we will apply the acoustically treated liner condition at duct walls and study its implementation in the time domain and the associated numerical stability.

ROBERTO MARSILIO

Interaction of homogeneous turbulence with a 3D shock wave

A fundamental understanding of compressible turbulence is necessary for the development of supersonic transport aircraft. Compressibility effects on turbulence were found to be significant when the energy associated with the dilation fluctuations is large or when the mean flow is significantly distorted (expanded or compressed). The presence of shock waves is an important feature that distinguishes high-speed from low-speed flows. Understanding the mechanisms of homogeneous turbulence interacting with a shock wave is not only of generic interest, but also of fundamental importance in understanding the interactions of turbulent boundary layers with shock waves which occur in many practical engineering applications: the flow inside a high speed compressor or a gas turbine, the flow over wings in supersonic aircraft, and the intake flow to a supersonic ramjet.

Numerical simulation using turbulence models is becoming a standard tool in aerospace technology. Most current models of compressible turbulence are, however, based on incompressible concepts. A better understanding of the underlying physics could lead to improvements in turbulence models, leading to more efficient designs. There is, therefore, a need to assess our understanding of compressible turbulence. This research was conducted in collaboration with G. Erlebacher.

The numerical approach is based on the time-dependent integration of the fully three-dimensional Navier-Stokes equations. The governing equations written in the quasi-linear form where the spatial derivatives are computed using a 6th order compact scheme while the time integration is performed

by a 4th order Runge-Kutta scheme. The shock is fitted using a three-dimensional shock-fitting procedure in which the shock is treated as moving internal boundary separating two (upstream and downstream) regions. To simulate shock turbulence interaction, we initialize the upstream flow (supersonic part) by superimposing homogeneous turbulence on the mean flow.

The code has been validated for three-dimensional flows and a numerical study of the effects of vortex stretching is in progress. The final goal of this work is to better understand the behavior of turbulence with particular regard to the shock/turbulence interaction.

JAMES E. MARTIN

A test of a vortex method for the computation of flap side edge noise

Upon approach to landing, a major source location of airframe noise occurs at the side edges of the part span, trailing edge flaps. In the vicinity of these flaps, a complex arrangement of spanwise flow with primary and secondary tip vortices may form. In the present study, we numerically investigate flap edge noise using a simple numerical model of the side edge flow field. A numerical procedure has been developed which incorporates the Lagrangian approach of a vortex method into a calculation for the noise radiated by a flow-surface interaction. A primary objective of the present study is to explore the viability of a Lagrangian technique like vortex methods for the prediction of noise radiation in situations of flow-surface interactions.

The noise generated by a vortex in the presence of a flat half plane is first considered. This problem serves as a basic model of flap edge flow. Furthermore, it permits the direct comparison between our computed results and the previous acoustic analyses of Hardin. One advantage of the vortex approach is that surface pressures may be obtained with exceptional resolution. We take advantage of this by numerically integrating the Ffowcs Williams-Hawkings equation to obtain the far field acoustic pressure.

In the future, the numerical procedure developed in this study will be applied to the case of a rectangular flap of finite thickness and ultimately modified for application to the fully three-dimensional problem. This work has been done in collaboration with J.C. Hardin. A similar investigation of sound radiation by free surface, shear layer flows is also currently being addressed (see F.Q. Hu).

NIMAI K. MITRA

Effect of exit boundary condition on large-eddy simulation of channel flows

Large-eddy simulations are generally performed by using periodic boundary conditions at the inlet and exit. This corresponds to fully developed or periodically fully developed flows. In many practical applications, e.g., in impinging jets, periodic boundary conditions (BC) are impractical. Investigation of the effects of nonperiodic boundary conditions provided the motivation of our work.

Together with my doctoral students T. Czesla and H. Laschefske, finite volume codes for DNS and LES (with Smagorinsky Lilly SGS) were developed for incompressible impinging jets. We have tested our LES code to simulate fully developed turbulent flow in a channel. To test the effect of exit BC, we computed the first half of the channel with periodic BC and the second half with exit BC of

constant pressure and vanishing first gradients. We considered two cases: (a) equidistant grids and (b) the last ten cells before the channel exit increasing successively 10% in length. Comparison of results with exit BC and fully developed flow (periodic BC) shows that the results with elongated cells differ less than 6% and the results with equidistant cells differ 10% from the fully developed values.

The boundary condition with elongated cells will be tested with impinging jets. However, further modification for the flow entrainment will be necessary.

DEMETRIUS T. PAPAGEORGIOU

Breakup of liquid jets

Liquid jets arise in numerous technological applications including printing, spraying processing of materials, fuel injection systems. The breakup process is desirable in some applications (as those above) but not so in others such as extrusion processes in fiber optics manufacturing. The dynamics governing breakup are fundamental and a full study of the breakup mechanisms has been undertaken.

The approach is a mixture of modeling, analysis of the resulting nonlinear systems and numerical computations. The breakup of a jet into droplets is nonlinear and in addition it manifests itself mathematically as a finite-time localized singularity of the governing equations, whether these are the Euler, Stokes or Navier-Stokes systems. We have analyzed all these systems and have constructed similarity solutions which give universal breakup for viscous jets. Reduced systems of equations have been derived and analyzed in an attempt to produce simpler models which have the basic physical mechanisms. The results are very encouraging for both viscous and inviscid jets.

Future plans include (i) direct numerical simulations to verify the nonlinear similarity solutions, (ii) extension to two-phase jets in the study of breakup control, (iii) addition of surface active agents such as those present in common inks or propulsion systems in order to model more realistically the variations of surface tension with the state of the system. In addition the program will be extended to compressible jets and also flows with a swirl component.

J. RAY RISTORCELLI

Compressible turbulence modeling

We are interested in creating a consistent set of models for the effects of compressibility. These effects include variable inertia effects associated with variations in the mean density, the mass flux, and effects due to the non-zero fluctuating dilatation.

The focus of the research has been on the dilatational covariances which act to convert the kinetic energy of the turbulence into internal energy. Primary focus has been on the reversible transfer due to pressure dilatation which is also the dominant mechanism in flows with important velocity gradients. The dilatational dissipation has been found to be of secondary importance in flows with important turbulence production mechanisms.

The theoretical aspects of the effects of the nonzero fluctuating dilatation for flows amenable to a pseudo sound theory, are now complete. In addition to the direct effects of compressibility

on the turbulent kinetic energy equation, rational expressions for the effects of compressibility on the eddy-viscosity have also been obtained. Analytical results indicate compressibility can increase or decrease the eddy-viscosity depending on the local values of the production, dissipation and turbulent Mach number. This will help develop simpler eddy-viscosity closures. The results of the analysis have been tested in a self-similar as well as parabolic mixing layer; the severe decrease in mixing layer growth as indicated by the well-known (if only suggestive) “Langley curve” is found. Effects of the model in nonequilibrium Mach 7 (J. White) flows indicate better agreement with experimental data.

Future plans in this area will address the investigation of additional implications of the analytical work. An algebraic stress closure has been derived for the effects of compressibility: we shall update this formalism following Girimaji’s extension of the theory. Codes to test the model and compare it to flows such as the jet – in which the pressure dilatation suppresses turbulence energy and the wake in which the pressure dilatation enhances the kinetic energy are in progress.

Eddy-viscosity transport models in compressible flows

In compressible flows with large mean density gradients the usual eddy-viscosity/gradient transfer models for the turbulent transport in both the $k - \epsilon$ and second-order closure methods appear to be inadequate. As a result, corrections, due to the presence of mean density gradients, of eddy viscosity transport expressions used to model turbulent transport of $\{u_i u_j\}_{,k}$ and ϵ are under investigation.

A direct investigation and order of magnitude analysis of various higher order Favre-moment equations for compressible flows with large density variations has shown this to be the case. An analysis carefully accounting for the distinction between Favre and Reynolds averaged quantities in the moment equations has identified the problem. An implementation of these ideas shows better agreement for simple equilibrium wall-bounded flows.

Additional and more conclusive experimental data with which to test the ideas are being sought.

Additional effects of compressibility

A nontrivial extension of the theory for the dilatational covariances mentioned above, to flows that have substantial mean density gradients or heat transfer effects is in progress. The work has been suggested by the poorly understood effects of heat transfer on the spread rates of hot jets; and the need to remove some of the limitations of the pseudo-sound theory. These issues, applied to the mixing problem of jet plumes, have been reported in some of the investigations on the effects of temperature on the spread rate of heated jets by J. Seiner (NASA).

Preliminary results show the importance of the pressure flux and the mean pressure gradient on the sign and magnitude of the nonisentropic corrections to the dilatational covariances.

Progress in this area will be related to the resolution of several difficult issues associated with models for the pressure flux in compressible flows.

ROBERT RUBINSTEIN

Evaluation of correlations in compressible turbulence

The Mach number and Reynolds number dependence of certain single point correlations are required for the computation of compressible turbulent flow. Correlations containing the dilatation are particularly significant as they enter the energy equation explicitly and provide the simplest manifestations of compressibility effects. This work was done in collaboration with G. Erlebacher.

In theories of weakly compressible turbulence, such correlations can be reduced to correlations of an incompressible background state of turbulence. Such correlations were evaluated in Fourier space to exploit the possibility of simple convergence tests which lead without any assumptions to the correct Reynolds number dependence. Using this method, and invoking the weakly compressible theory recently proposed by J.R. Ristorcelli, we calculate two correlations dependent on the dilatation and find for the ratio of compressible to incompressible energy the ratio $M^4 Re^{1/2}$ and for the ratio of compressible to incompressible dissipation the ratio $M^4 Re^{-1/2}$.

It is proposed to extend this calculation to another weakly compressible theory due to Zank and Matthaeus.

Free convective turbulence

A wide variety of applications require models for turbulent free convection. The appearance of a coupled fluctuating field, namely the temperature, complicates standard approaches based on closing single point moments and increases the difficulty of direct simulation. Analytical theories are a plausible starting point for such problems. This work was done in collaboration with Y. Zhou.

Following methods recently proposed by Woodruff, inertial range similarity solutions are developed for the direct interaction approximation equations for free convection. They provide preliminary estimates for inertial range constants which appear in turbulence models. A dissipation rate transport equation has been derived for free convection based on these methods. The correct form for this equation remains somewhat controversial in the modeling community.

It is proposed to complete this model by computing the somewhat less accessible production terms. An extension of the model to low Prandtl number flow is also envisioned.

Sound radiation by isotropic turbulence

Lilley's recent re-evaluation of Proudman's formula for the sound radiated by isotropic turbulence has called attention to this problem, a solution to which is needed when direct simulation of sound radiated by turbulence is not feasible. This work was done in collaboration with Y. Zhou.

We have re-evaluated Lilley's computation using inertial range formulas for turbulent correlations. For time correlations, both the hypothesis of dominant sweeping interaction and the hypothesis of dominant straining interaction were considered. The results generally agree with Lilley in suggesting that the "Proudman constant" is flow-dependent; however, the Strouhal number dependence found by Lilley is somewhat modified.

Further investigation of experimental and simulation data is needed to help decide between the sweeping and straining hypotheses.

SUTANU SARKAR

Modeling of compressible, reacting turbulence

We are interested in the simulation and modeling of compressible reacting flows. The effect of compressibility and high heat release on the evolution of the turbulent flowfield and on the mixing of fuel with reactant is our primary focus.

DNS of isotropic turbulence with hydrogen/air combustion has been conducted for a range of Mach numbers. It appears that, for such a flow, large heat release does not have an appreciable effect on the volume-averaged statistics of the velocity and its derivatives. However, the evolution of the conserved, reacting scalar pdf is somewhat different from that of a passive scalar. The DNS database is being used to improve the modeling of scalar mixing in collaboration with S. Girimaji.

The theoretical modeling will be continued with the DNS providing guidance and validation. Variable density and dilatational effects in reacting flow will be explicitly accounted for in the new models.

PATRICIA L. SHAH

Fluid-structure-acoustic interaction of a vortex and an edge of an elastic plate

Aircraft cabin noise is caused by a number of sources. The component believed to make a substantial contribution to interior cabin noise of a jet transport in steady cruise is boundary layer generated noise. As a result, it is the subject of intense experimental scrutiny and numerical modeling. Numerical schemes for predicting boundary layer generated interior noise must take proper account not only of sound waves produced by the fluid-structure interaction, but also of structural vibration generated by the flow that can subsequently generate sound by interacting with structural inhomogeneities. Such predictions must ultimately be validated by comparison with experiment, but it is useful to have available a collection of benchmark analytic solutions against which the numerical results can be compared.

CHARLES G. SPEZIALE

Time-dependent RANS

An analysis of new methodologies to develop improved Reynolds stress models suitable for Reynolds-averaged Navier-Stokes (RANS) computations of statistically unsteady turbulent flows was undertaken with B.A. Younis, S.A. Berger and Y. Zhou.

Particular attention is being placed on the addition of time-dependent/nonlinear terms in the representation for the Reynolds stress tensor and on the modeling of the dissipation rate tensor within a two-equation model format. Care will be taken to ensure that the model chosen is consistent with a full second-order closure in the equilibrium limit of homogeneous turbulence. This will allow for the incorporation of many of the good physical features of second-order closures within the framework of a more computationally robust two-equation model.

Applications to the time-dependent vortex shedding past bluff bodies – which is important from an aerodynamic standpoint – are envisioned.

Modeling of turbulent diffusion

A more systematic approach for the modeling of the turbulent diffusion terms in the Reynolds stress transport equation was investigated in collaboration with B.A. Younis and T.B. Gatski (LaRC) in order to develop improved models.

This approach is based on an analysis of the transport equation for the triple velocity correlation tensor. Models will be obtained in the equilibrium limit via integrity bases methods from linear algebra. To the lowest order, these models reduce to the commonly used gradient transport models. However, the new models will account for more turbulence physics than those based on gradient transport.

Applications of the new models to diffusion dominated turbulent flows are planned. These flows include jets, wakes and mixing layers which are of aerodynamic importance. This effort has the potential to lead to substantially improved full Reynolds closures for aerodynamic applications.

SIVA THANGAM

Development and validation of turbulence models for incompressible and compressible flows

The work described concentrates on the development of efficient turbulence models for incompressible and compressible flows as well as their validation. In this context, high Reynolds number flows of practical interest are analyzed by modeling turbulent stresses with two-equation anisotropic models that have wide range of predictive capability. The work performed during the current semi-annual period involves collaborative efforts with Y. Zhou, R. Ristorcelli, M.Y. Hussaini, T. Gatski (NASA), K.R. Rajagopal (University of Pittsburg) and A. Mahalov (Arizona State University).

The analysis of incompressible flows was performed using three different two-equation models. These include: a) the recursion renormalization group theory (r-RNG) based anisotropic two-equation model, b) an algebraic representation of a well-known second-order closure model, and c) a generalized turbulence model based on extended thermodynamics. All three models were implemented and tested using an efficient finite-volume code for the prediction of turbulent separated flows past a backward-facing step. The investigations show that all three models are equally efficient and are well-suited for modeling complex turbulent flows of general engineering applicability. The work in progress includes the implementation of r-RNG based near-wall model with consistent energy spectrum for wall-bounded flows as well as the analysis of wake flows and internal flows in conduits. Investigations on the development and implementation of two-equation models based on the algebraic representation of a recently developed second-order closure for compressible turbulence were also undertaken during the current period. The model utilizes both pressure-dilatation and dilatational-dissipation for kinetic energy and has been successfully applied for wall-bounded flows and supersonic mixing layers. This effort will be continued to include wake flows and other complex turbulent flows of aerodynamic relevance.

In addition, a turbulence model for rotating flows is under development based on phenomenological treatment of the rotation-modified energy spectrum. While the solid body rotation influences the energy transfer process significantly, it does not enter the kinetic energy equation explicitly. A dissipation rate equation with rotation rate dependent model coefficients has been developed. The model is currently being calibrated and will be applied to rotating duct flows using a r-RNG theory

based closure. This effort, involving compressible as well as incompressible turbulent flows, will be continued.

LU TING

Structural/acoustic interaction problem

The structural/acoustic interaction problem is essential for the prediction and control of panel fatigue and the transmission of external acoustic waves through panels of an airframe into the interior. We study the experimental data obtained by L. Maestrello at NASA LaRC on the interaction of incident acoustic waves, turbulent boundary layer and panel oscillations and the effectiveness of an active control device on the panel oscillation and the transmitted wave. It was found that the panel response and the transmitted wave for a steady flow are completely different from those for an accelerating flow. Theoretical studies were carried out for the interaction problem where the medium is moving at a constant velocity, subsonic or supersonic. But for a medium moving at an unsteady velocity $U(t)\hat{i}$, explicit solution for the acoustic field and its comprehensive study are not available. In collaboration with F. Bauer (Courant Institute, New York University) and L. Maestrello (NASA), we made a systematic study of wave propagation in a medium moving at an unsteady velocity. A summary of this work is:

In the interaction of an acoustic field with a moving airframe we encounter a canonical initial value problem for an acoustic field induced by an unsteady source distribution, $q(t, \mathbf{x})$ with $q \equiv 0$ for $t \leq 0$, in a medium moving with a uniform unsteady velocity $U(t)\hat{i}$ in the coordinate system $\mathbf{x}$ fixed on the airframe. Signals issued from a source point S in the domain of dependence $\mathcal{D}$ of an observation point P at time t will arrive at point P more than once corresponding to different retarded times, τ in the interval $[0, t]$. The number of arrivals is called the multiplicity of the point S . The multiplicity equals 1 if the velocity U remains subsonic and can be greater when U becomes supersonic. For an unsteady uniform flow $U(t)\hat{i}$, rules are formulated for defining the smallest number of I subdomains V_i of $\mathcal{D}$ with the union of V_i equal to $\mathcal{D}$. Each subdomain has multiplicity 1 and a formula for the corresponding retarded time. The number of subdomains V_i with nonempty intersection is the multiplicity m of the intersection. The multiplicity is at most I . Examples demonstrating these rules are presented for media at accelerating and/or decelerating supersonic speed.

Currently, we are developing a numerical program implementing the above theoretical results. For a given unsteady velocity $U(t)$, the program will define the domains of integration V_j and compute the retarded time τ_j for a point in a V_j . This program depends only on $U(t)$ but requires the input of the acoustic source distribution. The next step is to identify the source distribution, which can be a theoretical or numerical model, or data from experiments. Thus we can compare the acoustic fields induced by the same source distribution moving with different velocity function $U(t)$, to demonstrate the effect of unsteadiness and compare with experimental measurements of the acoustic field.

PETER R. VOKE

Large-eddy simulation: models, methods and implications

We investigate the theory and implementation of local backscatter in large-eddy simulations (LES) of turbulence.

The theoretical aspects of the modeling were accomplished rapidly and completed in one week. The work of Carati et al. was used as a basis and led directly to tests using a random vector potential to produce stochastic forcing fields that were (i) divergence-free (ii) localized in space and (iii) controlled in energy content. It was not possible to implement or test this formulation for localized backscatter in a dynamic subgrid scale model in a real LES since this would have required extensive Cray cpu resources; the testing will be done in England. In addition, many discussions on methods for LES were carried out with ICASE personnel including T. Gatski, B. Younis, G. Erlebacher, B. Rubinstein, J. Morrison, Y. Zhou and V. Venkatakrishnan; and on implications for modeling, with J.R. Ristorcelli. These discussions led to further computational work on the efficient implementation of compact difference schemes on vector supercomputers and a small number of preliminary tests were carried out on the Sabre (YMP) machine at the end of the second week. A seminar presented at ICASE also led to additional discussions.

A more extended visit will allow for the running of real LES on NASA supercomputers, testing the dynamic localization model with localized stochastic backscatter. The practicality of high-accuracy compact schemes for LES using general covariant Navier-Stokes will also be investigated.

ROBERT V. WILSON

Simulation of complex, three-dimensional turbulent jets

Three-dimensional, turbulent jets issuing from elliptic or rectangular nozzles exhibit many complex phenomena including strong azimuthal instabilities, switching of major and minor axes, and increased entrainment rates leading to increased mixing. The objective of the present work is to perform numerical simulations of these flows in order to understand such phenomena.

The study will include Large Eddy and Direct Numerical Simulations of rectangular jets issuing from nozzles and orifices and circular jets with vorticity generating tabs. A numerical formulation has been developed which uses high-order, compact finite differences for spatial derivatives and a low-storage, Runge-Kutta formulation for time advancement. The formulation has been validated by successfully solving a number of 1-d and 2-d benchmark problems ranging from a simple convection equation to the Navier-Stokes equations. The results of these tests verify that sixth-order convergence of the spatial error can be achieved with grid refinement.

Future efforts will focus on transforming the numerical formulation to a curvilinear coordinate system. Simulation of the above mentioned jets can then be performed and compared with the existing numerical and experimental studies.

STEPHEN L. WOODRUFF

Large-eddy simulation of a non-equilibrium periodic turbulent shear flow

The sheer enormity of the computational task of a complete simulation of fully-developed fluid-mechanical turbulence has led to the development of many approximate approaches for getting less complete answers at a smaller cost. One such approach is large-eddy simulation, in which the larger scales of motion are computed explicitly and the smaller scales are represented in only a very general way by a turbulence model. This turbulence model is clearly central to the success of the approach, and as one seeks to compute increasingly complex flows, one expects to need increasingly sophisticated models. At the suggestion of M.Y. Hussaini, some new turbulence models were applied to the large-eddy simulation of a periodic turbulent shear-flow problem proposed by NASA scientist J. Shebalin.

The new turbulence models under investigation were previously developed using ideas from the analytical theory of turbulence and are specifically designed to improve the simulation of non-equilibrium turbulent flows by incorporating history effects into the description of the small-scale motion. The spectral code developed by Dr. Shebalin for the direct numerical simulation of his periodic shear-flow problem was converted to a code for large-eddy simulations by changing the time-stepping algorithm to allow for the spatially-dependent eddy viscosity and by incorporating the turbulence models into the equations of motion.

The code developed in this work permits the turbulent flow to be driven over a wide range of length scales, with arbitrary time histories. This capability will allow the determination of conditions under which the new turbulence models provide a useful improvement over the models currently in use.

JIE-ZHI WU

Reduced laminar and turbulent stress tensor

The stress tensor appears in the momentum equation of fluid dynamics through a divergence, of which the outcome is a vector with at most three independent components, no matter how many components the stress tensor has. This simple observation implies that it is always possible to replace the stress tensor by a simpler one, the best having only as many independent components as its divergence has. This reduction may bring significant saving in analysis and computation.

We showed that the desired reduced stress tensor can be constructed from the Stokes-Helmholtz (S-H) decomposition. This is first exemplified by the reduced laminar stress tensor for Navier-Stokes flow with constant shear viscosity. The turbulence stress tensor, no matter what model is used, can be similarly reduced, of which a general formula is given in wave-number space. Moreover, we found that by using the helical-wave decomposition (HWD) the reduced tensor can be further simplified.

This work was done in collaboration with Y. Zhou and J.M. Wu.

Vorticity alignment in homogeneous turbulence

In small-scale turbulence, there is strong numerical evidence that the vorticity tends to align with the intermediate eigenvector of the strain-rate tensor. Some theoretical interpretation has been made, but one needs to further clarify whether this is a pure kinematic effect or some dynamics is involved. More quantitative theoretical estimate is also desired.

Owing to its beautiful intrinsic nature, the helical-wave decomposition (HWD) is an ideal mathematical tool for studying vorticity dynamics in wave-number space. In terms of HWD, we showed that the intermediate eigenvector of the strain rate takes the simplest form, so that for homogeneous turbulence we were able to formulate a simple criterion for the most probable alignment, which holds if the turbulence is also isotropic. This kinematic result is further sharpened by an HWD dynamic analysis, which leads to a necessary and sufficient condition for the most probable alignment in any homogeneous turbulence.

We plan to carry out some numerical test on our new criterion. This work was done in collaboration with Y. Zhou, D.D. Wu, and X.H. Wu.

Helical-wave decomposed Lamb vector in weakly compressible flow

The Lamb vector is the key nonlinear quantity that bridges the longitudinal and transverse dynamic processes in fluid motion: its divergence is the source of sound or shock wave, while its curl governs the evolution of vorticity field. In so doing, the Lamb vector itself is affected by both processes. The Lamb vector is also one of the central concerns in turbulence theory and modeling. It is therefore of great value to carry out a thorough analysis of various phases of the Lamb vector.

We used the helical-wave decomposition (HWD) to study the behavior of the Lamb vector in a weakly compressible flow, the simplest model flow to exhibit the longitudinal-transverse interaction. The power and neatness of HWD analysis has been illustrated in our above-mentioned studies. The results include a detailed display of the structure of the Lamb vector. In particular, as the source of vortex-sound, that structure analysis gives a theoretical guidance of noise control.

Based on this and the above progress, we plan to develop models for anisotropic turbulence, in particular near a solid wall or a free surface. The HWD will be utilized to simplify the formulation. This work was done in collaboration with Y. Zhou, D.D. Wu, and X.H. Wu.

PUI-KUEN YEUNG

Spectral transfer in rotating turbulence

Recent studies in the literature indicate that strong rotation causes turbulence to become quasi two-dimensional, through modification of the energy transfer between the large and small scales. However, the details of this process are not well understood, and similarly, little is known about the spectral transfer of scalars in rotating turbulence. Our objective is to perform direct numerical simulations (DNS) of isotropic turbulence subjected to rotation, and to use the resulting high-resolution databases to study detailed interscale energy and scalar transfer, including the relative roles of local versus nonlocal interactions. This work is performed in collaboration with Y. Zhou.

A number of 64^3 simulations with uniform solid-body rotation have been performed with a massively parallel DNS code for initially stationary isotropic turbulence, at Taylor-scale Reynolds

number ($Re_\lambda = 38$) in the presence of forcing at the large scales. Linear growth of the turbulence kinetic energy is observed after a transient period. A trend towards two-dimensionalization is evident through the growth of velocity fluctuations perpendicular to the rotation vector, but increased integral length scales measured along the latter. Analysis of energy transfer in the DNS database demonstrates explicitly that in the plane perpendicular to the rotation vector, the forward energy cascade due to nonlocal interactions is greatly reduced. In fact, a relatively local inverse cascade is observed, which leads to increasing concentration of energy in the large scales. In turn, the latter leads to great statistical variability, which necessitates ensemble averaging to be taken over multiple independent realizations for accurate statistics. Preliminary results for passive scalars indicate similar trends towards two-dimensionality.

The presence of a wide range of scales is important in the study of spectral transfer. Accordingly, we have submitted a proposal to NASA Langley for significant parallel computer time on the 160-node IBM SP2. We plan to conduct 256^3 simulations at $Re_\lambda = 150$, for which a short inertial range is expected in the energy spectrum. In addition, 128^3 simulations of scalar transport at $Re_\lambda = 90$ are proposed.

BASSAM A. YOUNIS

Rational modeling of the triple velocity correlations in second order closures

In contrast to other agencies in the exact equation for the Reynolds stresses, turbulent transport has received little attention from the turbulence-modeling community on the basis that this term is generally small and that existing models for the triple velocity correlations are adequate. Neither belief is generally true: turbulent transport is important in a whole class of weakly-sheared flows (e.g., wakes) and may well be the root cause of the plane jet/round jet anomaly. The existing models are for the most part mere perturbations of the simple gradient-transport hypothesis and they fail badly in asymmetric flow conditions (e.g., in mixing layers).

We proposed a new model for the triple velocity correlations – based not on closure of their exact transport equations but, rather, on postulating a functional relation for these correlations and then developing this with the aid of group representation theory. The resulting model contains all known existing models as sub-sets. Moreover, the gradients of mean velocity appear explicitly in the new formulation – an initially unexpected result but one which is clearly implied by the exact transport equations.

Work is now in progress in collaboration with C.G. Speziale (Boston University) and T.B. Gatski (NASA) aimed at finalizing the form of the model prior to calibrating it using LES/DNS data. Benchmarking the model against data from a number of practically-relevant shear flows will then follow.

Development of non-linear algebraic model for the turbulent scalar fluxes

Existing models for the turbulent scalar fluxes, both algebraic and differential, fail badly in complex turbulent fields; the former due to oversimplification of the relation between the fluxes and the mean velocity and scalar fields and the latter due to inadequate modeling of the fluctuating pressure-scalar gradient correlation term. The objective of this work was to advance an improved algebraic representation for the turbulent scalar fluxes.

This was achieved in collaboration with C.G. Speziale and T. Clark (Los Alamos National Laboratory). A nonlinear algebraic model for the turbulent scalar fluxes was developed with the use of representation group theory. The model is very simple, being of the gradient-transport variety, yet it contains all the necessary dependencies that are necessary for the correct prediction of the scalar field in complex turbulence. Thus, gradients of mean-velocity (that are absent from conventional gradient-transport models) are present and so are the turbulent stresses themselves. There is also a term which contains a product of the mean scalar- and velocity-gradients; the presence of which is suggested by the exact solution of the fluctuating pressure-scalar gradient correlations.

The calibration of this model using DNS data for the scalar fluxes in free and wall-bounded flows is now in progress. Also in progress is collaborative work with J. Shebalin (NASA) based on the use of his DNS code to study the evolution of the turbulent scalar fluxes in various strain fields.

CHARLES ZEMACH

An isosceles approximation to a spectral turbulence model

Spectral turbulence models of the Eddy-Damped Quasi-Normal Markovian (EDQNM) type take account of the non-locality of triad interactions in wave-number space. The evolution rate of the energy spectrum is given by a double integral over variables denoting two sides of a wave-number triangle. Strictly local models produce results with greatly reduced computational effort, and so may have greater applicability for complex flows. Their accuracy relative to the double-integral models is satisfactory in some cases, but not in others. We propose to construct a middle-of-the-road model which, by simplifying the EDQNM integrand, yields an evolution equation defined by a single wave-number integral.

We exploit an interesting but little recognized fact of Euclidean geometry. Consider the two sides of an arbitrary triangle which are closest to each other in magnitude. Then their ratio cannot exceed unity by more than 62% or be less than unity by more than 38%. Within this limited variable, “all triangles are essentially isosceles”. The double-integration region divides into three subregions, in each of which the energy density as a function of one wave number is approximated by the first two terms of a Taylor expansion in one of the other two wave numbers. The integrand’s dependence on the first wave number in its appropriate subregion is now algebraic and trivially integrable. The outcome is a simplified evolution equation which, it is hoped, is a good approximation to the EDQNM model.

We plan to explore the utility of this “isosceles” model by illustrative calculations with comparisons to both local and non-local spectral turbulence models.

YE ZHOU

Influences of subgrid scale dynamics on resolvable scale statistics in large-eddy simulations

Although direct numerical simulations (DNS) can be extremely useful in many areas related to the study of turbulence physics and the assessment of theories, it is restricted to relatively low Reynolds number (Re). Virtually all scientific and engineering calculations of nontrivial turbulent flows, at high Re , are based on some type of modeling. Large-eddy simulations (LES) are a logical ‘modeling extension’ of DNS. In LES, the three-dimensional time-dependent motion of these large scales are computed directly while the small scales are modeled (the so called ‘subgrid scale modeling’ problem). It is desirable to develop subgrid models based on systematical approaches.

Recently, the ϵ -expansion and recursive-renormalization group (RNG) theories as well as approximation inertial manifolds (AIM) are exploited as a systematic approach to subgrid modeling. Although these theoretical approaches are rather complicated, their key approximations can be investigated using direct numerical simulations. In fact, the differences among these theories can be traced to whether they keep or neglect interactions between the subgrid-subgrid and subgrid-resolvable scales. We focussed attention on the influence of these two interactions on the evolution of the resolvable scales. Indeed, our analysis leads to two interesting LES models: First, the LES^A model which keeps only the interactions between the small and large scales; the LES^B model, on the other hand, keeps only the interactions between the subgrid-subgrid scales. The performance of these models is analyzed using the velocity fields of the direct numerical simulations (DNS). Specifically, our comparison is based on the analysis of the energy and enstrophy spectra, as well as higher-order statistics of the velocity and velocity derivatives. We found that the energy spectrum and higher-order statistics of the LES^A are in very good agreement with the filtered DNS. The comparison between the LES^B model and the filtered DNS, however, is not satisfactory. Moreover, the decorrelation between the filtered DNS and LES^A is much slower than that of the filtered DNS and LES^B . Therefore, we conclude that the LES^A model, taking into account the interactions between the subgrid and resolvable scales, is a faithful subgrid model for LES. This work was done in collaboration with T. Dubois and F. Jauberteau (Laboratoire de Mathématiques Appliquées, Université Blaise Pascal and CNRS (URA 1501), France).

We plan to develop a subgrid model in physical space, based on our LES^A model tested here in spectral space.

YOUSEF H. ZURIGAT

On the accuracy of triple-deck solution for compressible boundary layers

The asymptotic triple-deck theory has been in use for predictions of mean flow and its stability in both incompressible and compressible boundary layers over bodies with surface imperfections, suction through porous strips, compression ramps and others. Although satisfactory performance of the triple-deck method was established in the incompressible flow case, the theory in its first and higher order forms was found to be less satisfactory in the compressible flow case. In this latter case, recent studies suggest that the triple-deck theory has serious limitations. It was argued that the first-order linear triple-deck theory is merely the first term in an asymptotic expansion of the Orr-Sommerfeld equations governing the stability of compressible boundary layers. Consequently

the theory should give results that are less accurate than those obtained by solving the full equations governing the stability problem.

In this summer visit, we looked into this problem (in collaboration with M.Y. Hussaini and G. Erlebacher) and a dispersion relation for the stability of compressible boundary layer over a flat plate was derived from the viscous Orr-Sommerfeld equations specialized for the lower deck in the triple-deck structure as a first term asymptotic expansion in powers of $Re^{-\frac{1}{8}}$. Independently, Erlebacher obtained a general dispersion relation from the first order linear triple-deck theory which when applied to the flat plate compressible flow case resulted in an identical result. Preliminary results of the neutral stability curve using the full linear stability Orr-Sommerfeld equations and the dispersion relation mentioned above were obtained for a Mach number of 0.8. Although the disagreement was found to be large, no concrete statement regarding this result can be stated as this time as further tests need to be carried out first. This is ongoing.

Further work will include the study of this problem by application to different two- and three-dimensional instability modes in two-dimensional compressible boundary layers.

APPLIED COMPUTER SCIENCE

DAVID C. BANKS

Animation and interpolation of vortices in unsteady flow

We display vortical features from flow data using a parallel computer in order to interpolate the surface geometry between known time steps and produce animated visualizations of the flow dynamics.

We represent vortex tubes as generalized cylinders using a truncated Fourier-series radius function to describe the cross-sections. With this representation we can conveniently interpolate between shapes at successive time steps, as long as the topology of a tube does not change.

We use the Parallel Graphics Library (PGL) on the Intel Paragon to interpolate the vortex tube and render high-resolution images into an animation file.

Visualization of this time-varying data set helps the scientist see the dynamics at work in the flow being studied. We are developing techniques that will run at interactive speeds for the workstation-class machines of the future.

We are developing techniques to visualize velocity in a single, static frame of data by adding dynamics to small-scale deformations of the geometry of features in the data. We are also tackling the problem of interpolating geometry across changes in the topology of the vortices.

SHAHID H. BOKHARI

Communication overhead on Paragon, SP2 and CS-2

Interprocessor communication overhead is a crucial measure of the power of a parallel processing system — its impact can severely limit the performance of parallel programs. This work is concerned with evaluating communication overhead on three contemporary commercial multicomputer systems. These are the Intel Paragon at Caltech, the IBM SP2 at Cornell and the Meiko CS-2 at Vienna.

Detailed measurements have been made on these three machines of (1) the time to communicate between two processors, (2) synchronization time, and (3) memory access time. The impact of link contention has also been explored. The data obtained provide a valuable resource for researchers in analyzing the performance of their parallel programs on these three machines.

Future work shall address other commercial architectures and shall attempt to investigate in detail the impact of contention on multistage networks.

Multiphase complete exchange on Paragon, SP2 and CS-2

The complete exchange is the severest communication pattern that can be required of a parallel computer system. It requires each of n processors to send a distinct message to all other $n - 1$ processors. This pattern is at the heart of many important parallel algorithms such as the Alternating Direction Implicit method (ADI), FFTs, distributed table lookups, etc. On hypercubes,

multiphase complete exchange has been developed and shown to provide optimal performance over varying message sizes.

This research has explored the implementation of multiphase complete exchange on the Intel Paragon, IBM SP2 and Meiko CS2. These contemporary machines do not have hypercube interconnects. They do, however, have high performance interconnection networks and can be shown to emulate hypercubes reasonably well. It has been shown that the theoretical ideas developed for hypercubes are also applicable in practice to these machines. Multiphase complete exchange can lead to major savings in execution time over traditional solutions.

In the future this work will be extended to other architectures and the algorithm already developed will be enhanced to better take into account the special communication hardware of specific machines.

Bounded contention complete exchange on meshes

Direct algorithms for complete exchange send each message block to its destination in one "direct" transmission. An optimal direct algorithm is one that requires $n - 1$ transmissions on an n processor system. Such an algorithm has been known for hypercubes for some time. On mesh-connected parallel computers David Scott has developed an algorithm that requires $n^{(3/2)}/4$ transmissions and shown it to be the best possible under the assumption that only one message can occupy a communication link at one time. This work was conducted in collaboration with D. Nicol.

On the Intel Paragon mesh, the bandwidth of communication links is greater than the rate at which processors can inject messages into the communication network. Thus it is possible to send two or more messages through a link with minor penalty. Bounded contention complete exchange is an extension of Scott's algorithm that develops a schedule in which contention on links is bounded by a given integer. This algorithm has been developed and implemented on the Intel Paragon. It has been established that this algorithm leads to major advantages over naive direct complete exchange algorithms.

It is expected that this work will be extended to higher-dimensional meshes and to non-mesh architectures. We are also interested in unifying this algorithm with the multiphase algorithm.

XIAO-CHUAN CAI

Parallel performance of a Newton-Krylov-Schwarz algorithm

We implemented a Newton-Krylov-Schwarz algorithm on the Langley IBM SP2, with the MPL communication library, for solving the 2D full potential equation of aerodynamics. The partial differential equation is discretized with a bilinear finite element method with density upwinding in the supersonic regions.

We solve the full potential equation with a modified transpiration boundary condition that simulates the symmetric NACA0012 airfoil. Our solution, i.e., the C_p curve, agrees nicely with the solution obtained by using the Boeing TRANAIR code at least for the subsonic case. Our current effort is on the understanding of the proposed algorithm for the transonic case.

We plan to further study this class of parallel algorithms for the full potential equation and later use it as part of the preconditioners for a parallel Euler/Navier-Stokes solver. This work is being done in collaboration with D. Keyes.

TZI-CKER CHIUEH

Parallel volume rendering for time-varying data sets

Rendering time-varying volumetric data sets poses a different problem than rendering static volumetric data. To improve the overall throughput, the resources of a parallel system must be effectively utilized. In particular, the I/O overhead of parallel volume rendering must be masked as much as possible. This work is being performed jointly with K.-L. Ma.

We started with a naive approach by repeating the execution of a generic parallel volume renderer on the time-varying sequence of 3D data sets, and found that during the beginning and the end of the rendering process for a single data set, the nodes are mostly idle, thus wasting resources. To address this problem, we try to pipeline the rendering tasks for consecutive data sets in the sequence, essentially exploiting inter-volume as well as intra-volume parallelism. Given a fixed number of processor nodes and I/O bandwidth, the research question is what is the optimal balance between inter-volume and intra-volume parallelism exploitation. We have implemented a prototype volume renderer that embodies the idea of pipelined rendering for time-varying data sets. We are able to achieve the most effective system utilization bounded only by the I/O bandwidth. To reduce the I/O overhead, the current implementation exploits Intel Paragon's parallel I/O capability.

Currently, more detailed performance measurements are being collected and analyzed. Ultimately, we'd like to devise an automatic scheme to make the optimal tradeoff between inter-volume and intra-volume parallelism, based on the data size and the hardware capabilities. We also plan to extend the current system with the idea of asynchronous pipelining, where data subsets are tagged and passed among nodes as they traverse from I/O nodes, through computation nodes, to display nodes. With appropriate tagging, the synchronization delay among processing nodes can be completely eliminated.

GIANFRANCO CIARDO

Distributed analysis of discrete-state stochastic models

The state-space generation for stochastic models is often a critical step in their analysis. For large, complex models, the size of the data structures required to store the reachability graph greatly exceeds the capability of a single workstation.

We then propose to use a distributed approach, where the generation algorithm is run on a network of workstations, thus making available their overall memory and processing power. A key issue is how to split the reachability graph in such a way that it is allocated with a reasonable uniformity over the workstations. We use a "partitioning function," which, given a state, decides which process is responsible for it. At the end, the incidence matrix of the graph is stored by columns, in a distributed way, according to the partitioning function. We estimate the quality

of this function by the percentage of reachability graph arcs which are “cross-arcs” (they connect states in different processes), which cost in terms of communication, and by how uniformly spread the states are. We have an implementation running under Sun/Unix, and the speedup results (for up to six workstations) are promising.

So far, the modeler is charged with defining a good partitioning function. We plan instead to investigate an algorithm for the automatic generation of this function, given the properties of the particular model being studied. Also, the numerical solution of the process is currently still centralized. We plan to add a distributed solution in the near future. This work is being performed jointly with D. Nicol.

THOMAS W. CROCKETT

Parallel rendering algorithms for distributed-memory message-passing architectures

We are continuing the development of parallel rendering algorithms and associated software to provide runtime visualization support for parallel application programs.

Our recent work has focussed on scalability and load-balancing issues, including a detailed experimental study of the overheads which arise in practice. Our asynchronous sort-late rendering algorithm, coupled with a scanline-based static image decomposition scheme, performs well with up to 128 processors on the IBM SP2 and Intel Paragon. This result holds even for scenes with large spatial variations in image complexity. We have also been developing better algorithms for retrieving image segments and delivering them to external display devices. This has resulted in improved interactive performance, particularly on the SP2, which is able to fully utilize the available network bandwidth.

We plan to extend our performance studies to larger numbers of processors when such configurations become available to us and when the operating systems become sufficiently robust to support the algorithms.

PHILLIP M. DICKENS

Thread-based parallel direct execution simulator

Parallel direct execution simulation is an important tool for performance and scalability analysis of large parallel-message programs executing on top of a presumed *virtual computer*. In this approach the application code is executed directly to determine its run-time behavior, and any references to the presumed virtual computer are trapped and handled by simulator constructs. However, detailed simulation of message-passing codes requires a great deal of computation, and we are therefore interested in pursuing implementation techniques which can decrease this cost. This work is being done in collaboration with M. Haines, P. Mehrotra and D. Nicol.

Our approach is to implement the simulated virtual processors as light-weight threads rather than heavy-weight Unix processes thus reducing both on-processor communication costs and context switching costs. However, this approach brings up the important issue of how to provide the separate address spaces required for each of the simulated virtual processors when threads are generally implemented such that they all share one global address space. Our solution is to

implement the virtual processors using the C++ class mechanism which automatically provides the required separate address spaces. We have a preliminary version of our thread-based direct execution simulator implemented on a cluster of Sun workstations. Preliminary studies show that the thread-based simulator offers up to a ten-fold improvement in performance when compared to the process-based approach.

The performance results obtained thus far are from synthetic loads. Current research is aimed at implementing and testing large parallel application codes in order to obtain a true measure of the costs and benefits of this new approach.

MATTHEW HAINES

Runtime support for task and data parallelism

Integrating task and data parallelism requires sophisticated runtime support to handle issues of communication and synchronization among parallel tasks in an application, each of which may execute in a data parallel manner. Additionally, mapping these tasks onto a limited set of physical resources may require sharing resources among several tasks, which may or may not be related. Our objective is to design and implement a thread-based runtime system that can provide an efficient solution to the problems of integrating task and data parallelism. This work is being done in collaboration with P. Mehrotra, and ViLAP graduate fellow student D. Cronk.

We have divided the runtime project into two layers, a lower layer for supporting language-independent, lightweight threads capable of communication in a distributed memory environment (Chant), and a higher layer for providing the support required by the Opus language (Opus Runtime). We have designed and implemented Chant atop POSIX pthreads and MPI. In addition to supporting Opus Runtime, we are using Chant to determine the benefits of combining threads with data parallel compilers and scientific applications.

We plan to continue development of these two layers of the runtime system. We also plan to study lightweight threads in relation to load balancing, irregular scientific problems, and performance prediction and evaluation.

Smartfiles: An object-oriented approach to data file interoperability

Data files for scientific and engineering codes typically consist of a series of raw data values whose interpretation is buried in the programs that interact with these files. In this situation, where the meaning of a data file is implicit in associated programs, making even minor changes in the file structure or sharing file between programs (interoperability) can only be done by careful examination of the I/O statements of the programs using this file. Moreover, parallel changes are often required at many points in the system. By applying object-oriented techniques to files, we can add the intelligence required to improve data interoperability and provide an elegant mechanism for supporting complex evolving or multidisciplinary applications. This work is being done in collaboration with P. Mehrotra and J. Van Rosendale.

We have completed the preliminary design and prototype software system, and are currently working on extending the prototype to support the full functionality of the design.

We plan to continue development on the Smartfile system and study the performance characteristics of the system as compared with existing approaches. We also plan to start using the system for some of the application codes being used at ICASE.

JIM E. JONES

Parallel multigrid methods

Standard multigrid methods are not well suited for problems with anisotropic coefficients, which can occur, for example, on grids that are stretched in order to resolve a boundary layer. There are several different modifications to the standard algorithm that yield efficient methods for these problems. Which of these modifications results in the most efficient parallel algorithm is an open question.

Our work began with a survey of the existing literature on parallel multigrid methods, and the findings are summarized in the paper "Parallel Multigrid Methods", co-authored with S.F. McCormick. This paper will appear in the publication dedicated to the ICASE/LaRC Workshop on Parallel Numerical Algorithms. In addition to providing an overview of the many aspects of parallel implementation of multigrid methods, the article discusses several multigrid algorithms which are known to be robust with respect to anisotropic coefficients. These include those based on standard coarsening and alternating block relaxation, semi-coarsening and block relaxation, and multiple semi-coarsening. In the survey, we were unable to find any work comparing the efficiency of these algorithms on today's generation of parallel computers. We have begun designing and implementing codes based on these algorithms and variations of them, to investigate this question. The extension of these algorithms to non-uniform grids is itself an open research question, ignoring the added complexity introduced by parallel computing. Thus, we decided to restrict ourselves initially to structured grids. As such, the application appears to be well suited for use of High Performance Fortran (HPF), a FORTRAN based language for parallel computing. The HPF component of this project is done in collaboration with P. Mehrotra of ICASE.

Our plan is to implement several robust multigrid algorithms in HPF and analyze their performance on the parallel computers at Langley. Our primary goal is to answer questions about which algorithm is most efficient for particular applications. Our secondary goal is to answer questions about HPF's suitability as a language for developing parallel multigrid codes.

HARRY F. JORDAN

High speed radix sort for optoelectronic implementation

Some optoelectronic devices are capable of working at bit rates in excess of 100 Gigabits per second, but have constraints on latency and repetition rate. Radix sort can be formulated in such a way that it can take advantage of these devices in spite of their constraints. A target architecture for sorting a 16 way partitioned serial stream of numbers is being developed. It can potentially run at 1.6 Terabits per second, making it competitive with supercomputer sort speeds but with far less complexity.

The design uses fiber optics with high throughput optical exchange elements switching at the word rate to rearrange data order. The bitwise computation needed by radix sort is done by one high speed Nonlinear Optical Loop Mirror (NOLM) per stream. The data rearrangement kernel also forms a basis for fast Fourier transform computation. Algorithmic changes in this kernel have a strong impact on the number of expensive optical switches that are required.

We are moving toward a laboratory demonstration of the sorter. Current important problems involve optical signal restoration and synchronization. Partitioning the synchronization problem into bit level and word level sub-problems seems to be a promising approach.

Metrics for data movement requirements of parallel programs

The performance of a parallel program on a given architecture is strongly dependent on the demands for data movement among processors made by the program and on the ability of the architecture to satisfy them. The temporal nature of the demand is particularly important. Large volumes of irregular data movement over a short period are hard to achieve in hardware. Architecture independent metrics characterizing the data movement capacity a program needs to execute at full speed are sought.

Techniques based on a sliding time window on the interprocess data movement requests reveal communication time scales as the window size is varied. The method can be applied to explicitly parallel programs for either shared or distributed memory multiprocessors. Metrics are calculated from abstract program traces for real programs, and can be calculated directly for simple kernels.

We will compute metrics on representative benchmarks using traces produced by the MINT simulator. The metrics will be compared against execution times of the benchmarks on both MINT simulated architectures and real machines with different data transport capabilities to determine the predictive power of the metrics.

DAVID E. KEYES

Parallel algorithms of Newton-Krylov-Schwarz type

Newton-Krylov-Schwarz is a general framework for the parallel implicit computation of PDEs in distributed environments. It combines a Newton-Krylov (NK) method, such as nonlinear GMRES, with a Krylov-Schwarz (KS) method, such as additive Schwarz. The linkage is the Krylov method, whose most important characteristic, from a parallel computational point of view, is that information about the underlying Jacobian needs to be accessed only in the form of matrix-vector products in a relatively small number of directions. Communication for this task is limited to nearest neighbor, with whatever (modest) overlap is needed to complete computational stencils that lie near processor boundaries. However, if the Jacobian is ill-conditioned, the Krylov method will require an unacceptably large number of iterations. The system can be transformed through the action of a preconditioner whose inverse action approximates that of the Jacobian, but at smaller cost. It is usually in the choice of preconditioning that the battle for low computational cost and scalable parallelism is won or lost. In KS methods, the preconditioning is introduced on a subdomain-by-subdomain basis, providing well load-balanced data locality for parallel implementations over a wide granularity range. A two-grid-level form of additive Schwarz provides a mesh-independent

and granularity-independent convergence rate in elliptically dominated problems, including non-symmetric and indefinite problems. As such, additive Schwarz can be regarded as a restricted form of multigrid, and a conventional multigrid can also be used within each subdomain to obtain a complexity per iteration whose only superlinear contribution is in the distributed coarse grid solve, itself.

NK technology has been demonstrated in a structured full potential code, structured and unstructured Euler codes, and in an unstructured Navier-Stokes code, where, as a serial solver, it generally trails multigrid by relatively small ratios of CPU time. Our CFD experiences are driving the development of the Argonne National Laboratory parallel Portable Extensible Toolkit for Scientific Computing (PETSc), through close interactions with its developers. We are currently running PETSc on workstation clusters, and on the LaRC Paragon and SP2. Collaborators in these projects include X.-C. Cai of UC-Boulder, M.D. Tidriri and V. Venkatakrishnan of ICASE, W.K. Anderson of LaRC, and W.D. Gropp, L.C. McInness, and B.F. Smith of Argonne. Collaborators on related NKS or NK demonstrations include D.A. Knoll and P.R. McHugh of INEL on non-premixed combustion problems, and D.P. Young and R.G. Melvin of Boeing on aerodynamic design problems.

Thus, a variety of CFD applications are (or have inner) nonlinear elliptically-dominated problems amenable to solution by NKS algorithms, which are characterized by relatively low storage requirements (for an implicit method) and locally concentrated data dependencies. The main disadvantage of NKS algorithms is the large number of parameters that require tuning. Parametric tuning and the trade-off between parallel scalability and preconditioner strength will continue as the main foci of our research.

Communication modeling in distributed computing

The “hyperbolic model” for communication costs in multi-layer contended networks is a two-parameter model that represents a practical compromise between communication models of greater fidelity, like the five-parameter LogGP model, and unrealistically ideal models, like the PRAM. Like the Bulk Synchronous Processors (BSP) model, the hyperbolic model is practical for distributed computations with a relatively small number of communication templates, such as broadcast, global reduction, and nearest neighbor exchange.

Since its introduction, the hyperbolic model has been related to established models, such as the linear $(r_\infty, n_{1/2})$ model of Hockney and Jesshope and the LogP model of the Berkeley NOW group. Upon expressing the hyperbolic model parameters in terms of the parameters of these other models, we have shown that the hyperbolic model has the same large message asymptote as the $(r_\infty, n_{1/2})$ model and is within 25% of the small message limit of the LogP model, while doing better for small messages than the $(r_\infty, n_{1/2})$ model and for large messages than the LogP model, with monotonically varying departures for messages of intermediate size. Since typical scientific and engineering codes require messages of diverse sizes (ranging from scalar floats in inner products to full planes or volumes of data in whole-grid transfers in time-parallel methods), such robustness with respect to message size for a small number of parameters, namely two, is highly desirable.

Instrumented prototype PDE-based codes using MPI primitives are now being run to evaluate the hyperbolic model parameters on diverse architectures available at LaRC.

SCOTT T. LEUTENEGGER

Data base support for subset retrieval and visualization of scientific data

To design and implement a prototype database to facilitate retrieval of subsets of large scientific data sets. The data subsets are anticipated to be used as inputs to other codes, such as for visualization or MDO.

Currently many scientists store and retrieve data sets as files. When the scientist is interested in a subset of the data they read in the entire data set and strip out the portion of interest. This is not practical when data sets are large. Our approach is to provide database support to retrieve only those pages from disk that contain the desired data. Typical CFD data sets are two or three dimensional, thus we provide multi-attribute indexing techniques.

During an eight week visit to ICASE we continued development of our prototype by focusing on support for irregular grids. We implemented 2D and 3D Rtrees, and devised and implemented new efficient bulk loading algorithms for 2D Rtrees. The Rtrees and bulk loading algorithms provide us with a unified format for both block structured and irregular grids.

We will continue development of the prototype next fiscal year by completing algorithms for efficient loading of 3D Rtrees and interfacing with visualization routines. Integration with visualization will be carried out in collaboration with K.-L. Ma.

KWAN-LIU MA

3D visualization of shock wave on unstructured grids

In this research, we are investigating ways of displaying a three-dimensional shock wave so its location and topology clear. Determining the exact location and structure of the shock wave is not at all trivial, in particular, on unstructured grids. One problem is that due to errors in the numerical approximation of the fluid dynamics equations, shocks are ordinarily smeared over several grid cells. Moreover, the data is available only at the vertices of the grid, which do not coincide with the exact shock location, so interpolation issues arise.

Once the shock is found, there is the issue of appropriately displaying the shock in three dimensions. Typically, the flow field discontinuity will form a surface, which can be displayed using such visualization techniques as lighting or smooth shading. In order to convey its location relative to the airfoil or other aircraft structure, the shock surface may be rendered with partial transparency. Another option is to use volume-rendering related techniques, which display the shock as a fuzzy cloud using overlapping partially transparent objects.

Our research results suggest that multiple shock-wave detection schemes and visualization methods are needed for data of different characteristics. This research was done in collaboration with W. Vermeer and J. Van Rosendale.

Out-of-core visualization on unstructured grids

Computational modeling of scientific and engineering problems can produce very large amount of data. Most of the existing visualization tools such as FAST, AVS, Fieldview, etc. handle data efficiently only when the data can fit into the main memory of the computer used. Moreover, unstructured grids introduce additional complications and difficulties into the visualization processes. There are generally two approaches for visualizing large data sets. One is to make use of a massively parallel computer or a cluster of workstations. The other is to do out-of-core calculations; that is, the main memory is loaded on demand with only a portion of the total data.

In this research, we have started by developing algorithms and data structures for performing out-of-core visualization of unstructured-grid data. Our algorithms has been designed according to the characteristics of unstructured grids and visualization algorithms, as well as the cpu, disk and network performance. A visualization process consists of three steps: data partitioning, visualization calculations and displaying. Data partitioning is based on an octree subdivision scheme and needs to be done only once for a particular computing environment. Visualization calculations are optimized by taking advantage of spatial coherence and data sharing as much as possible.

The current prototype system can draw streamlines, streamribbons, streamtubes, iso-surfaces and volume rendered images. Regardless the size of the data, all visualization, except volume rendering, can be made at an interactive rate. We have done tests for measuring the performance of the algorithms and implementation by using data sets of sizes ranging from several hundred thousands to several million tetrahedra on a single Sun workstation. The test results show the feasibility of our design. Future work includes the development of better graphical user interface and porting the current design to a parallel distributed-memory computing environment. This research is being conducted in collaboration with S.K. Ueng and D. Mavriplis.

PIYUSH MEHROTRA

Software environment for multidisciplinary applications

Several of the Grand Challenge problems require the integration of independently executing modules into a larger coordinated application to solve the problem at hand. For example, multidisciplinary design of an aircraft requires codes for airflow analysis, structural analysis, performance analysis, etc., to work in concert in order to produce an optimal design. From the point of view of software, this entails support not only for the control and coordination of the individual discipline codes and but also for the sharing of data between these codes. This work is being done in collaboration with M. Haines, J. Van Rosendale, B. Chapman and H. Zima.

We have designed a set of language extensions, called Opus, which provide such support. The central concept in Opus is that of a ShareD Abstraction (SDA), a set of data structures along with methods to access the data. Methods can be activated asynchronously or synchronously and each method, when executing, has exclusive access to the data. SDAs can be used as computation servers to encapsulate the individual discipline codes. They can also be used as data repositories for communicating and sharing data between the computation servers. The SDAs can be internally data parallel; we rely on HPF directives inside SDAs to express such parallelism. We have implemented a prototype system which encodes the protocols necessary for supporting method activation and

exclusivity. The prototype also handles arguments distributed using HPF directives. This prototype currently runs on a network of homogeneous workstations or on an MPP such as the Intel Paragon or the IBM SP2.

We plan to continue evaluating the language design, modifying it as necessary based on our evaluation. We also plan to extend the runtime system to run across a heterogeneous network of architectures including both workstations and MPPs. We plan to base this implementation on Chant, the thread based portable language independent system that we are also developing.

Evaluation of HPF

The stated goal of High Performance Fortran (HPF) was to “address the problems of writing data parallel programs where the distribution of data affects performance.” We have been using data parallel codes of interest to NASA to evaluate the effectiveness of the language features of HPF. This work is being done in collaboration with the graduate students K. Roe and K. Winn.

In the last six months, we have used four compilers for this evaluation: APR’s compiler on the Intel Paragon, PGI’s compiler on the Intel Paragon and the IBM SP2, DEC’s compiler on the DEC Alpha Farm and IBM’s (beta) compiler on the SP2. These compilers have varying degrees of maturity and optimizations built into them. We have used a simple parallel loop to measure the efficiency of the code generated by these compilers. We are also continuing our experiments with the model version of the multiblock code TLNS3D. By distributing each block of data onto individual processors, we have obtained excellent speedups in the flux computations of TLNS3D. The boundary exchange routine had runtime dependencies and takes a large fraction of the total time. By restructuring the code drastically, we have been able to cut down the time considerably for the PGI compiler on the Paragon. The results of our experiments have been communicated both to the HPF Forum and to the compiler vendors.

In the next six months, we plan to evaluate different distribution strategies for TLNS3D with at least the APR and the PGI compilers. We also plan to investigate the effort required to parallelize the full TLNS3D code along with other codes of interest to NASA.

DAVID NICOL

Utilitarian parallel simulator

One of the principal reasons that parallel discrete event simulation has not made an impact on simulation practice is the difficulty of programming the synchronization correctly. Our objective is alleviate this problem in the context of simulating parallel computer and communications systems. This research was conducted in conjunction with P. Heidelberger (IBM).

Our approach recognizes that several successful conservative synchronization algorithms are known to be effective in the context of simulating parallel computer and communication systems. We have developed a software library called U.P.S. (Utilitarian Parallel Simulator) that is used in conjunction with the commercial CSIM simulator package, to provide transparent synchronization and communication. The simulation modeler develops models largely as he would for a serial simulation. By incorporating U.P.S. constructs at the interface between simulation processes, the synchronization and communication activity is carried out automatically. U.P.S. has been implemented on the Paragon, and on the IBM SP-2. Recent work includes basing it on MPI rather than

nx, extending its functionality by adding more sophisticated lookahead features, and performance tuning.

Future plans include extending it further to accept direct-execution measurements as input.

Threaded application parallel system simulator (TAPS)

System software that supports threads is difficult to develop because there numerous design decisions whose impact cannot be forecast without implementation and experimentation. Our objective is to develop a simulation tool that will be used as part of the system software design process, in order to reduce the effort needed to make rationale design decisions.

Our approach has been to develop the Threaded Application Parallel System Simulator (TAPS). TAPS has been restructured to implement the execution-driven functional simulation paradigm. TAPS supports different policies with regard to scheduling and polling for messages. TAPS is written in C++ and uses CSIM; its design supports easy extension to other workload and communication network models.

Our plans for the future are to parallelize TAPS using U.P.S., to expand the types of thread scheduling policies it supports and to develop more sophisticated interfaces to it, e.g., supporting the Ports0 functionality in TAPS models.

ALEX POTHEN

Graph partitioning algorithms

Many computational problems in scientific computing are governed by an underlying graph (e.g., finite element meshes that represent discretized partial differential equations). When algorithms for these problems are obtained by applying the divide and conquer paradigm, or when parallel algorithms are designed for such problems, the graph needs to be partitioned into a specified number of subgraphs such that the number of edges joining different subgraphs is small.

In earlier work, we had designed an algebraic algorithm for partitioning graphs that relies on an eigenvector of the Laplacian matrix of the graph. The attempt to obtain a fast implementation of this algorithm led to the design of a multilevel algorithm for graph partitioning. In this algorithm, we compute from the given graph a sequence of coarser graphs until the coarsest graph is small enough (typically a few hundred vertices). The coarsest graph is then partitioned, and the partition projected to the next finer graph in the sequence. The projected partition is then refined by a Kernighan-Lin algorithm that swaps subsets of vertices to improve the quality of the partition. The projection and refinement of the separators are repeated until a partition of the finest graph in the sequence (the initial graph) is obtained. This algorithm was initially implemented by Hendrickson and Leland at Sandia National Labs. We have implemented a variant of this multilevel algorithm for computing nested dissection orderings in the context of parallel sparse matrix factorization. We are now investigating an algorithm that is efficient when the graph is partitioned into several subsets by recursive graph bisection.

After completing an efficient implementation, we will apply the partitioning algorithm to solve sparse systems of equations in parallel. We will consider the partitioning of anisotropic problems, and develop a parallel implementation. We will also study the quality of partitions computed by multilevel methods. The criteria for preferring one graph partition over other depends strongly on

the application: we will consider other criteria for optimization, and a general-purpose algorithm that can deal with different optimization criteria.

Envelope reduction of sparse matrices

Frontal algorithms for solving large, sparse, systems of linear equations require the matrix to be reordered to reduce a parameter called the wavefront of the matrix. Iterative solvers require the reduction of the envelope size of the associated coefficient matrix in order to compute good preconditioners. We have designed new combinatorial and algebraic (spectral) algorithms for wavefront and envelope reduction. This work has applications to the gene sequencing problem in computational biology.

An improved hybrid algorithm for envelope and wavefront reduction, which combines the good “global” framework of a spectral ordering with the muscle of a “local” combinatorial ordering has been developed in the past year with my graduate student Gary Kumfert. Our results show that the hybrid algorithm can (1) reduce the envelope parameters significantly over other algorithms, and (2) calculate the ordering faster than a spectral algorithm, since the expensive eigenvector can be computed to lower precision. The algorithm has shown to be effective in frontal factorization methods for structural analysis on a Cray Y-MP, and in computing preconditioners.

We are now focusing on the fast computation of wavefront-reducing orderings by reducing the complexity of the combinatorial algorithm. We will also apply our techniques to ordering unsymmetric matrices, and anisotropic problems.

A Microeconomic scheduler for parallel computers

Scheduling the jobs arriving at a parallel (cluster) computer such that the mean response time of a job is small, while the system utilization is high, is an important problem in the current computational milieu. We are continuing our work on a novel scheduling algorithm based on a microeconomic paradigm in which job priorities depend on the amount of “money” a user has. This is joint work with I. Stoica and H. Abdel-Wahab, both at Old Dominion University.

Our simulation results on test data from log files of jobs submitted at NASA Ames Research Center and Argonne National Laboratory show that our scheduler improves both system and user performances in comparison with two current scheduling policies, particularly when the work load is high. The improvements range from 20 to 40% depending on the system load. Furthermore, our algorithm can deal with the issues of fairness and user control of the performance of a user’s jobs. This work was presented at a Workshop on Job Scheduling at the International Parallel Processing Symposium, and will appear in a volume of Springer Verlag’s Lecture Notes in Computer Science.

In current work, we are studying a variant of the scheduling algorithm which sets job priorities based on a queuing model used in communication networks. This expectation is that this variant of the scheduler should be analytically tractable, and thus its performance on realistic test data can be predicted. We will also further develop the scheduling algorithm for use in the parallel and cluster computing community.

AHMED SAMEH

Parallel algorithms for block tridiagonal linear systems

Numerous science and engineering applications give rise to large block tridiagonal linear systems of equations. Efficient parallel algorithms for solving such systems are often vital for the efficient implementation of codes of these applications on parallel architectures. This work is being done in collaboration with Vivek Sarin.

Several parallel direct algorithms are available in the literature for solving such linear systems. Some of these algorithms have been developed by the author and his collaborators. During this one week at ICASE, a survey of direct schemes, as well as iterative schemes with parallel preconditioners, has been initiated. In the process of launching this survey, we have improved several preconditioned iterative schemes.

The parallel direct schemes are based on a partitioning (or a divide-and-conquer) strategy. An algorithm in this class has been studied extensively on shared memory parallel machines, where data locality allowed us to overcome the potential disadvantages of arithmetic redundancy. For iterative schemes, we refined a domain decomposition-based approach for solving such systems for the symmetric positive definite and general cases. In addition, we refined a preconditioned block-row projection scheme for handling such systems. We plan to present numerical experiments on the Cray T3D, a network of SGI workstations, and a cluster-based shared memory multiprocessor.

ARUN K. SOMANI

Large simplified phased-mission system analysis for independent component-based systems

Accurate analysis of reliability of system requires that it accounts for all major variations in system's operation into account. Most reliability analyses assume that the system configuration, success criteria, and component parameters remain the same or can be described using simple distributions. However, multiple phases are natural in many missions. In such cases, the failure/repair rates of components, system configuration, and success criteria may vary, and therefore, must be accounted for appropriately. At the same time efficiency in computation must be maintained.

We developed a new computationally efficient technique for phased-mission analysis of systems where the behavior of a system can be described using a fault tree and components include no repairs. We are currently improving on that work to allow repairs on individual components as long as the component repairs are independent of system state. The repair is carried out depending on the component state only. In such cases, the behavior of a system can still be described using combination logic (such as fault tree or assertions). We are also developing a method to simplify the computation. Our technique avoids state space explosion that commonly plague Markov chain-based analysis while accounting for the effects of variable configurations and success criteria from phase to phase. Our technique yields exact results.

After refining this technique, we will implement this in a reliability analysis tool. This is part of our broader research in developing specification methods, languages, and tools for an Integrated Modeling and Analysis System.

XIAN-HE SUN

Performance evaluation of parallel algorithms and architectures

As parallel machines with more and more processors becoming available, the performance metric *scalability* is becoming increasingly important. Most of scientific applications are “scalable” in the sense that larger problems will be solved when more computational power is available. Scalability measures how an algorithm, a machine architecture, and an algorithm-machine combination will perform when problem size is scaled up linearly with computing power (number of processors) in a parallel and distributed system. Because of its importance, intensive research has been conducted in recent years in scalability study. However, scalability has been traditionally studied separately. Its relation with execution time has not been revealed. Time is the ultimate measure in practice. Scalability study would only have limited practical impact if it cannot provide sufficient information of the variation of execution time in a scalable computing system.

The relation between scalability and execution time is carefully examined in current study. Theoretical analysis are applied for general applications. Three parallel algorithms are developed and tested on two parallel platforms, Intel Paragon and IBM SP2, to confirm the theoretical findings. Theoretical and experimental results show that isospeed scalability is a good indicator of time variation when problem and system size are scaled up. For any pair of Algorithm-Machine Combinations (AMC) that have the same initial execution time, an AMC has a smaller scalability if and only if it has a larger execution time on scaled problems; the same scalability will lead to an equal execution time, and vice versa. The relation is also extendible to more general situations where the two AMCs have different initial execution times. Scalability is an important companion and a good complement of execution time. Initial time and scalability together will describe the expected performance on larger systems.

Scalability study has practical importance in performance debugging, compiler optimization, and selection of an optimal algorithm/machine pair for an application. We have shown that initial time and scalability together will describe the expected performance of algorithms on a larger system. In the future, we would like to extend the study to actual simulation packages arising in CFD applications, in which multiple algorithms and multiple data structures exist, and performance prediction is more involved.

MOULAY DRISS TIDRIRI

Schwarz-based methods in CFD

Our goal is to develop and study optimal two-level Schwarz/MUSCL type algorithms, which are intended for the parallel implicit solution of aerodynamics problems.

Our investigation of Schwarz-based methods in CFD has continued. Both theoretical and practical aspects were addressed. From practical point of view, implementations and comparisons of several Schwarz-based approaches on 2D and 3D compressible flows were performed. From theoretical point of view, we have studied several Schwarz/MUSCL type schemes.

We are planning to further refine both our theoretical and numerical analysis of Schwarz-based methodologies.

KISHOR TRIVEDI

Fluid stochastic petri nets

One of the difficulties encountered while using Petri nets is that the reachability graph tends to be very large in practical problems. If this is due to an accumulation of large number of tokens in one or more places of the net, we can approximate the number of tokens in such places by continuous quantities. Drawing a parallel with fluid flow approximations in performance analysis of queuing systems, we can define such nets. Alternatively, some physical systems have not previously admitted a Petri net modeling approach, as they explicitly contain continuous fluid-like quantities which are controlled with discrete logic. This paper presents a new methodology for modeling such systems.

We introduce a new class of stochastic Petri nets in which one or more places can hold fluid rather than discrete tokens. Fluid can be thought of as approximating large numbers of tokens, or as representing actual continuous quantities in modeled systems. We define a class of fluid stochastic Petri nets in such a way that the discrete and continuous portions may affect each other through an intuitive extension of transition firing rules. Following this definition we provide equations for their transient and steady-state behavior. We present several examples showing the utility of the construct in communication network modeling, and reliability analysis, and discuss important special cases. We then discuss numerical method for solving for transient and steady-state behavior of such nets. Finally, some numerical examples are presented.

Equations describing the dynamics of such nets are partial differential equations. More work will continue exploring numerical methods of solution and applications of these new type net. The work is carried out jointly with G. Horton (Erlangen University), D. Nicol (ICASE) and V. Kulkarni (University of North Carolina at Chapel Hill).

Accelerated convergence of Markov chain calculations

Computing the mean time to failure (MTTF) in Markovian models of highly dependable systems can be computationally expensive, even for models with small state spaces, because of the slow rate of convergence. We seek to speed up such calculations by solving alternative sets of equations having much faster convergence rates. This work is being done in collaboration with P. Heidelberger.

Standard calculation of the MTTF involves solving a single set of linear equations. In our formulation, we solve a related set of equations with $(N + 1)$ different right hand sides. The equations and the right hand sides are obtained by selecting N “operational” states to be added to the set of failure states, where N can be set by the user. In a short second phase, the MTTF is then computed by solving a system of N equations. My earlier experimental work with $N = 1$ resulted in several orders of magnitude speedup for a variety of models. By using $N > 1$, we seek to broaden the class of models for which the method produces significant speedups. We have proven that the convergence rate is improved using this method and have developed heuristics for selecting which operational states to select.

We plan further experimentation on the method.

LINDA WILSON

Automated load balancing in parallel discrete-event simulation

Parallel discrete-event simulation offers the potential for significant speedup over sequential simulation. Unfortunately, high performance is often achieved only after rigorous fine-tuning is used to obtain an efficient mapping of tasks to processors. In practice, good performance with minimal effort is often preferable to high performance with excessive effort.

We have modified the SPEEDES simulation framework to automate static load balancing. Using simulation models of queuing networks and the National Airspace System, we have demonstrated that using run-time measurements, our automated load-balancing scheme can achieve better performance than simple allocation methods that do not use run-time measurements, particularly when large numbers of processors are used.

We are currently examining modifications to our system that will improve the performance of a distributed simulation. For future work, we will examine automated dynamic load balancing and the related issue of object migration. This work is performed in collaboration with D. Nicol.

Automatic tuning of parallel simulation control parameters

In parallel discrete-event simulation, performance is often dependent upon several user-defined parameters. For example, should the synchronization protocol be optimistic, conservative, or a hybrid of the two? Should the sending of messages be risky or risk-free? Should lazy or aggressive cancelation of messages be used? The optimal settings for these parameters will depend upon the simulation model and the current status of the parallel environment.

In the SPEEDES simulation framework, a small set of parameters controls the degree of optimism in the synchronization protocol. We have added performance monitors to SPEEDES to collect information on the effects of using different values for the individual control parameters.

Using these performance monitors, we will investigate the tuning of the control parameters using a controller which will be developed using ideas from control systems theory. We will merge this controller with SPEEDES and evaluate its performance on an Intel Paragon, a network of workstations, and a Sun SPARCcenter 2000. This work is in collaboration with R. Chamberlain (Washington University, St. Louis).

REPORTS AND ABSTRACTS

Dando, Andrew, and Philip Hall: *Wavenumber selection for small-wavelength Görtler vortices in curved channel flows*. ICASE Report No. 95-21, April 6, 1995, 28 pages. Submitted to *Studies in Applied Mathematics*.

We consider the problem of wavenumber selection for fully nonlinear, small-wavelength Görtler vortices in a curved channel flow. These type of Görtler vortices were first considered by Hall & Lakin (1988) for an external boundary layer flow. They proved particularly amenable to asymptotic description, it was possible to consider vortices large enough so that the mean flow correction driven by them is as large as the basic state, and this prompted us to consider them in a curved channel flow as an initial application of the phase-equation approach to Görtler vortices. This involves the assumption that the phase variable of these Görtler vortices varies on slow spanwise and time scales, then an analysis of both inside and outside the core region, to which vortex activity is restricted, leads to a system of partial differential equations which we can solve numerically for the wavenumber. We consider in particular the effect on the wavenumber of the outer channel wall varying on the same slow spanwise scale as the phase variable.

Ristorcelli, J.R.: *A pseudo-sound constitutive relationship for the dilatational covariances in compressible turbulence: An analytical theory*. ICASE Report No. 95-22, April 4, 1995, 50 pages. Submitted to the *Journal of Fluid Mechanics*.

The mathematical consequences of a few simple scaling assumptions about the effects of compressibility are explored using a simple singular perturbation idea and the methods of statistical fluid mechanics. Representations for the pressure-dilatation and dilatational dissipation covariances appearing in single-point moment closures for compressible turbulent are obtained. The results obtained, in as much as they come from the same underlying diagnostic relationship, represent a unified development for both the compressible covariances. While the results are expressed in the context of a second-order statistical closure they provide some interesting and very clear physical metaphors for the effects of compressibility that have not been seen using more traditional linear stability methods. In the limit of homogeneous turbulence with quasi-normal large scales the expressions derived are - in the low *turbulent* Mach number limit - asymptotically exact. The expressions obtained are functions of the rate of change of the turbulence energy, its correlation length scale, and the relative time scale of the cascade rate. With the appearance of the length scale the dilatational covariances are found to scale with the Mach numbers based on the mean strain and rotation rates. The expressions for the dilatational covariances contain constants which have a precise and definite physical significance; they are related to various integrals of the longitudinal velocity correlation. The pressure-dilatation covariance is found to be a non-equilibrium phenomena related to the time rate of change of the internal energy and the kinetic energy of the turbulence. Also of interest is the fact that the representation for the dilatational dissipation in a turbulence, with or without shear, features a dependence on the Reynolds number. cascade This article is a documentation of an analytical investigation of the implications of a pseudo-sound theory

for the effects of compressibility. The novelty of the analysis is in the very few phenomenological assumptions required to produce the results. Subsequent work will assess the consequences of this analysis in the context of compressible turbulence models for engineering calculations.

Shortis, Trudi A., and Philip Hall: *On the nonlinear stability of the unsteady, viscous flow of an incompressible fluid in a curved pipe*. ICASE Report No. 95-23, April 6, 1995, 23 pages. Submitted to the Journal of Fluid Mechanics.

The stability of the flow of an incompressible, viscous fluid through a pipe of circular cross-section, curved about a central axis is investigated in a weakly nonlinear regime. A sinusoidal pressure gradient with zero mean is imposed, acting along the pipe. A WKBJ perturbation solution is constructed, taking into account the need for an inner solution in the vicinity of the outer bend, which is obtained by identifying the saddle point of the Taylor number in the complex plane of the cross-sectional angle co-ordinate. The equation governing the nonlinear evolution of the leading order vortex amplitude is thus determined. The stability analysis of this flow to axially periodic disturbances leads to a partial differential system dependent on three variables, and since the differential operators in this system are periodic in time, Floquet theory may be applied to reduce this system to a coupled infinite system of ordinary differential equations, together with homogeneous uncoupled boundary conditions. The eigenvalues of this system are calculated numerically to predict a critical Taylor number consistent with the analysis of Papageorgiou (1987). A discussion of how nonlinear effects alter the linear stability analysis is also given, and the nature of the instability determined.

Sun, Xian-He, and Jianping Zhu: *Performance prediction: A case study using a multi-ring KSR-1 machine*. ICASE Report No. 95-24, April 6, 1995, 21 pages. To appear in the Proceedings of the 28th Hawaii International Conference on System Sciences, Jan. '95.

While computers with tens of thousands of processors have successfully delivered high performance power for solving some of the so-called "grand-challenge" applications, the notion of scalability is becoming an important metric in the evaluation of parallel machine architectures and algorithms. In this study, the prediction of scalability and its application are carefully investigated. A simple formula is presented to show the relation between scalability, single processor computing power, and degradation of parallelism. A case study is conducted on a multi-ring KSR-1 shared virtual memory machine. Experimental and theoretical results show that the influence of topology variation of an architecture is predictable. Therefore, the performance of an algorithm on a sophisticated, hierarchical architecture can be predicted and the best algorithm-machine combination can be selected for a given application.

Haras, Zigo, and Shlomo Ta'asan: *The large discretization step method for time-dependent partial differential equations*. ICASE Report No. 95-25, April 7, 1995, 53 pages. To be submitted to the Journal of Computational Physics.

A new method for the acceleration of linear and nonlinear time dependent calculations is presented. It is based on the Large Discretization Step (LDS, in short) approximation, defined in this work, which employs an extended system of low accuracy schemes to approximate a high accuracy discrete approximation to a time dependent differential operator. Error bounds on such approximations are derived. These approximations are efficiently implemented in the LDS methods for linear and nonlinear hyperbolic equations, presented here. In these algorithms the high and low accuracy schemes are interpreted as the same discretization of a time dependent operator on fine and coarse grids, respectively. Thus, a system of correction terms and corresponding equations are derived and solved on the coarse grid to yield the fine grid accuracy. These terms are initialized by visiting the fine grid once in many coarse grid time steps. The resulting methods are very general, simple to implement and may be used to accelerate many existing time marching schemes.

The efficiency of the LDS algorithms is defined as the cost of the computing the fine grid solution relative to the cost of obtaining the same accuracy with the LDS methods. The LDS methods typical efficiency is 16 for 2D problems and 28 for 3D problems for both linear and nonlinear equations. For a particularly good discretization of a linear equation an efficiency of 25 in 2D and 66 in 3D was obtained.

Mavriplis, D.J.: *Unstructured mesh generation and adaptivity*. ICASE Report No. 95-26, April 13, 1995, 47 pages. Lecture notes for 26th CFD Lecture Series of von Karman Institute; AGARD Publication.

An overview of current unstructured mesh generation and adaptivity techniques is given. Basic building blocks taken from the field of computational geometry are first described. Various practical mesh generation techniques based on these algorithms are then constructed and illustrated with examples. Issues of adaptive meshing and stretched mesh generation for anisotropic problems are treated in subsequent sections. The presentation is organized in an educational manner, for readers familiar with computational fluid dynamics, wishing to learn more about current unstructured mesh techniques.

Mavriplis, D.J.: *Multigrid techniques for unstructured meshes*. ICASE Report No. 95-27, April 13, 1995, 61 pages. Lecture notes for 26th CFD Lecture Series of von Karman Institute; AGARD Publication.

An overview of current multigrid techniques for unstructured meshes is given. The basic principles of the multigrid approach are first outlined. Application of these principles to unstructured mesh problems is then described, illustrating various different approaches, and giving examples of practical applications. Advanced multigrid topics, such as the use of algebraic multigrid methods,

and the combination of multigrid techniques with adaptive meshing strategies are dealt with in subsequent sections. These represent current areas of research, and the unresolved issues are discussed. The presentation is organized in an educational manner, for readers familiar with computational fluid dynamics, wishing to learn more about current unstructured mesh techniques.

Venkatakrishnan, V.: *Implicit schemes and parallel computing in unstructured grid CFD*. ICASE Report No. 95-28, April 13, 1995, 62 pages. Lecture notes for 26th CFD Lecture Series of von Karman Institute.

The development of implicit schemes for obtaining steady state solutions to the Euler and Navier-Stokes equations on unstructured grids is outlined. Applications are presented that compare the convergence characteristics of various implicit methods. Next, the development of explicit and implicit schemes to compute unsteady flows on unstructured grids is discussed. Next, the issues involved in parallelizing finite volume schemes on unstructured meshes in an MIMD (multiple instruction/multiple data stream) fashion are outlined. Techniques for partitioning unstructured grids among processors and for extracting parallelism in explicit and implicit solvers are discussed. Finally, some dynamic load balancing ideas, which are useful in adaptive transient computations, are presented.

Hall, Philip, and Demetrios T. Papageorgiou: *On the modulational instability of large amplitude waves in supersonic boundary layers*. ICASE Report No. 95-29, April 13, 1995, 44 pages. Submitted to SIAM.

The evolution of large amplitude Tollmien-Schlichting waves in a supersonic boundary layer is investigated. Disturbances which have their wavenumber and frequency slowly varying in time and space are described using a phase equation type of approach. Unlike the incompressible case we find that the initial bifurcation to a finite amplitude Tollmien-Schlichting wave is subcritical for most Mach numbers. In fact the bifurcation is only supercritical for a small range of Mach numbers and even then for only a finite range of wave propagation angles. The modulational instability of large amplitude wavetrains is considered and is shown to be governed by an equation similar to Burgers equation but with the viscous term replaced by a fractional derivative. A numerical investigation of the solution of this equation is described. It is shown that uniform wavetrains are unstable.

Mavriplis, D.J., and V. Venkatakrishnan: *A 3d agglomeration multigrid solver for the reynolds-averaged navier-stokes equations on unstructured meshes*. ICASE Report No. 95-30, April 13, 1995, 29 pages. Submitted to the International Journal for Numerical Methods in Fluids.

An agglomeration multigrid strategy is developed and implemented for the solution of three-dimensional steady viscous flows. The method enables convergence acceleration with minimal additional memory overheads, and is completely automated, in that it can deal with grids of

arbitrary construction. The multigrid technique is validated by comparing the delivered convergence rates with those obtained by a previously developed overset-mesh multigrid approach, and by demonstrating grid independent convergence rates for aerodynamic problems on very large grids. Prospects for further increases in multigrid efficiency for high-Reynolds number viscous flows on highly stretched meshes are discussed.

Crockett, Thomas W.: *Parallel rendering*. ICASE Report No. 95-31, May 10, 1995, 52 pages. To appear in "The Encyclopedia of Computer Science and Technology."

This article provides a broad introduction to the subject of parallel rendering, encompassing both hardware and software systems. The focus is on the underlying concepts and the issues which arise in the design of parallel rendering algorithms and systems. We examine the different types of parallelism and how they can be applied in rendering applications. Concepts from parallel computing, such as data decomposition, task granularity, scalability, and load balancing, are considered in relation to the rendering problem. We also explore concepts from computer graphics, such as coherence and projection, which have a significant impact on the structure of parallel rendering algorithms. Our survey covers a number of practical considerations as well, including the choice of architectural platform, communication and memory requirements, and the problem of image assembly and display. We illustrate the discussion with numerous examples from the parallel rendering literature, representing most of the principal rendering methods currently used in computer graphics.

Ta'asan, Shlomo: *Pseudo-time methods for constrained optimization problems governed by PDE*. ICASE Report No. 95-32, May 18, 1995, 15 pages. To be submitted to SIAM Journal on Optimization.

In this paper we present a novel method for solving optimization problems governed by partial differential equations. Existing methods use gradient information in marching toward the minimum, where the constrained PDE is solved once (sometimes only approximately) per each optimization step. Such methods can be viewed as a marching techniques on the intersection of the state and costate hypersurfaces while improving the residuals of the design equation per each iteration. In contrast, the method presented here march on the design hypersurface and at each iteration improve the residuals of the state and costate equations. The new method is usually much less expensive per iteration step, since in most problems of practical interest the design equation involves much fewer unknowns than either the state or costate equations. Convergence is shown using energy estimates for the evolution equations governing the iterative process. Numerical tests shows that the new method allows the solution of the optimization problem in cost equivalent to solving the analysis problem just a few times, independent of the number of design parameters. The method can be applied using single grid iterations as well as with multigrid solvers.

Stoica, Ion, Hussein Abdel-Wahab, and Alex Pothen: *A microeconomic scheduler for parallel computers*. ICASE Report No. 95-33, June 12, 1995, 23 pages. To appear in Proceedings of the Workshop on Job Scheduling Strategies for Parallel Processing, 9th International Parallel Processing Symposium.

We describe a scheduler based on the microeconomic paradigm for scheduling on-line a set of parallel jobs in a multiprocessor system. In addition to the classical objectives of increasing the system throughput and reducing the response time, we consider fairness in allocating system resources among the users, and providing the user with control over the relative performances of his jobs. We associate with every user a savings account in which he receives money at a constant rate. When a user wants to run a job, he creates an expense account for that job to which he transfers money from his savings account. The job uses the funds in its expense account to obtain the system resources it needs for execution. The share of the system resources allocated to the user is directly related to the rate at which the user receives money; the rate at which the user transfers money into a job expense account controls the job's performance.

We prove that starvation is not possible in our model. Simulation results show that our scheduler improves both system and user performances in comparison with two different variable partitioning policies. It is also shown to be effective in guaranteeing fairness and providing control over the performance of jobs.

Morano, E., D.J. Mavriplis, and V. Venkatakrishnan: *Coarsening strategies for unstructured multigrid techniques with application to anisotropic problems*. ICASE Report No. 95-34, May 31, 1995, 19 pages. To be submitted to SIAM Journal on Scientific Computing.

Over the years, multigrid has been demonstrated as an efficient technique for solving inviscid flow problems. However, for viscous flows, convergence rates often degrade. This is generally due to the required use of stretched meshes (i.e. the aspect-ratio $AR = \Delta y / \Delta x \ll 1$) in order to capture the boundary layer near the body. Usual techniques for generating a sequence of grids that produce proper convergence rates on isotropic meshes are not adequate for stretched meshes. This work focuses on the solution of Laplace's equation, discretized through a Galerkin finite-element formulation on unstructured stretched triangular meshes. A coarsening strategy is proposed and results are discussed.

Fahringer, Thomas, Matthew Haines, and Piyush Mehrotra: *On the utility of threads for data parallel programming*. ICASE Report No. 95-35, May 10, 1995, 14 pages. To appear in International Conference on Supercomputing '95.

Threads provide a useful programming model for asynchronous behavior because of their ability to encapsulate units of work that can then be scheduled for execution at runtime, based on the dynamic state of a system. Recently, the threaded model has been applied to the domain of data parallel scientific codes, and initial reports indicate that the threaded model can produce

performance gains over non-threaded approaches, primarily through the use of overlapping useful computation with communication latency. However, overlapping computation with communication is possible without the benefit of threads if the communication system supports asynchronous primitives, and this comparison has not been made in previous papers. This paper provides a critical look at the utility of lightweight threads as applied to data parallel scientific programming.

Haines, Matthew, Piyush Mehrotra, and David Cronk: *Ropes: Support for collective operations among distributed threads*. ICASE Report No. 95-36, May 10, 1995, 19 pages. Submitted to Supercomputing '95.

Lightweight threads are becoming increasingly useful in supporting parallelism and asynchronous control structures in applications and language implementations. Recently, systems have been designed and implemented to support interprocessor communication between lightweight threads so that threads can be exploited in a distributed memory system. Their use, in this setting, has been largely restricted to supporting latency hiding techniques and functional parallelism within a single application. However, to execute data parallel codes independent of other threads in the system, collective operations and relative indexing among threads are required. This paper describes the design of *ropes*: a scoping mechanism for collective operations and relative indexing among threads. We present the design of ropes in the context of the Chant system, and provide performance results evaluating our initial design decisions.

Carpenter, Mark H., and David Gottlieb: *Spectral methods on arbitrary grids*. ICASE Report No. 95-37, May 10, 1995, 29 pages. To be submitted to the Journal of Computational Physics.

Stable and spectrally accurate numerical methods are constructed on arbitrary grids for partial differential equations. These new methods are equivalent to conventional spectral methods but do not rely on specific grid distributions. Specifically, we show how to implement Legendre Galerkin, Legendre collocation, and Laguerre Galerkin methodology on arbitrary grids.

D'Ambrosio, Domenic, and Roberto Marsilio: *A numerical method for solving the three-dimensional parabolized Navier-Stokes equations*. ICASE Report No. 95-38, May 10, 1995, 24 pages. To be submitted to the Journal of Computational Physics.

A numerical technique that solves the parabolized form of the Navier-Stokes equations is presented. Such a method makes it possible to obtain very detailed descriptions of the flowfield in a relatively modest CPU time. The present approach is based on a space-marching technique, uses a finite volume discretization and an upwind flux-difference splitting scheme for the evaluation of the inviscid fluxes. Second order accuracy is achieved following the guidelines of the the ENO schemes. The methodology is used to investigate three-dimensional supersonic viscous flows over symmetric corners. Primary and secondary streamwise vortical structures embedded in the boundary layer and

originated by the interaction with shock waves are detected and studied. For purpose of validation, results are compared with experimental data extracted from literature. The agreement is found to be satisfactory, though some minor discrepancies appear, which nevertheless are difficult to be addressed to unaccuracies in the computations rather than to uncertainties in the experimental measurements. In conclusion, the numerical method proposed seems to be promising, as it permits at a reasonable computational expense to investigate complex three-dimensional flowfields in great detail.

Bauer, F., L. Maestrello, and L. Ting: *Acoustic field in unsteady moving media*. ICASE Report No. 95-39, May 10, 1995, 47 pages. Submitted to JASA.

In the interaction of an acoustic field with a moving airframe we encounter a canonical initial value problem for an acoustic field induced by an unsteady source distribution, $q(t, \mathbf{x})$ with $q \equiv 0$ for $t \leq 0$, in a medium moving with a uniform unsteady velocity $U(t)\hat{i}$ in the coordinate system $\mathbf{x}$ fixed on the airframe. Signals issued from a source point S in the domain of dependence $\mathcal{D}$ of an observation point P at time t will arrive at point P more than once corresponding to different retarded times, τ in the interval $[0, t]$. The number of arrivals is called the multiplicity of the point S . The multiplicity equals 1 if the velocity U remains subsonic and can be greater when U becomes supersonic. For an unsteady uniform flow $U(t)\hat{i}$, rules are formulated for defining the smallest number of I subdomains V_i of $\mathcal{D}$ with the union of V_i equal to $\mathcal{D}$. Each subdomain has multiplicity 1 and a formula for the corresponding retarded time. The number of subdomains V_i with nonempty intersection is the multiplicity m of the intersection. The multiplicity is at most I . Examples demonstrating these rules are presented for media at accelerating and/or decelerating supersonic speed.

Fitterman, A., E. Turkel, and V. Vatsa: *Pressure updating methods for the steady-state fluid equations*. ICASE Report No. 95-40, May 10, 1995, 15 pages. To appear in the Proceedings of the AIAA CFD Conference.

We consider the steady state equations for a compressible fluid. Since we wish to solve for a range of speeds we must consider the equations in conservation form. For transonic speeds these equations are of mixed type. Hence, the usual approach is to add time derivatives to the steady state equations and then march these equations in time. One then adds a time derivative of the density to the continuity equation, a derivative of the momentum to the momentum equation and a derivative of the total energy to the energy equation. This choice is dictated by the time consistent equations. However, since we are only interested in the steady state this is not necessary. Thus we shall consider the possibility of adding a time derivative of the pressure to the continuity equation and similar modifications for the energy equation. This can then be generalized to adding combinations of time derivatives to each equation since these vanish in the steady state. When using acceleration techniques such as residual smoothing, multigrid, etc. these are applied to the pressure rather than the density. Hence, the code duplicates the behavior of the incompressible equations for low speeds.

Bayliss, A., L. Maestrello, J.L. McGreevy, and C.C. Fenno: *Response of a multi-panel assembly to noise from a jet in forward motion*. ICASE Report No. 95-41, May 18, 1995, 29 pages. To appear at First CEAS/AIAA Aeroacoustics Conference.

A model of the interaction of the noise from a spreading subsonic jet with a 4 panel assembly is studied numerically in two dimensions. The effect of forward motion of the jet is accounted for by considering a uniform flow field superimposed on a mean jet exit profile. The jet is initially excited by a pulse-like source inserted into the flow field. The pulse triggers instabilities associated with the inviscid instability of the jet shear layer. These instabilities generate sound which in turn serves to excite the panels. We compare the sound from the jet, the responses of the panels and the resulting acoustic radiation for the static jet and the jet in forward motion. The far field acoustic radiation, the panel response and sound radiated from the panels are all computed and compared to computations of a static jet. The results demonstrate that for a jet in forward motion there is a reduction in sound in downstream directions and an increase in sound in upstream directions in agreement with experiments. Furthermore, the panel response and radiation for a jet in forward motion exhibits a downstream attenuation as compared with the static case.

Banks, H.T., R.C. Smith, D.E. Brown, R.J. Silcox, V.L. Metcalf: *Experimental confirmation of a PDE-based approach to design of feedback controls*. ICASE Report No. 95-42, May 19, 1995, 42 pages. Submitted to SIAM Journal of Control and Optimization.

Issues regarding the experimental implementation of PDE-based controllers are discussed in this work. While the motivating application involves the reduction of vibration levels for a circular plate through excitation of surface-mounted piezoceramic patches, the general techniques described here will extend to a variety of applications. The initial step is the development of a PDE model which accurately captures the physics of the underlying process. This model is then discretized to yield a vector-valued initial value problem. Optimal control theory is used to determine continuous-time voltages to the patches, and the approximations needed to facilitate discrete time implementation are addressed. Finally, experimental results demonstrating the control of both transient and steady state vibrations through these techniques are presented.

Zhou, Ye: *A phenomenological treatment of rotating turbulence*. ICASE Report No. 95-43, May 18, 1995, 13 pages. To appear in Physics of Fluids.

The strong similarity between the magnetohydrodynamic (MHD) turbulence and initially isotropic turbulence subject to rotation is noted. We then apply the MHD phenomenologies of Kraichnan and Matthaeus & Zhou to rotating turbulence. When the turbulence is subject to a strong rotation, the energy spectrum is found to scale as $E(k) = C_\Omega (\Omega \epsilon)^{1/2} k^{-2}$, where Ω is the rotation rate, k is the wavenumber, and ϵ is the dissipation rate. This spectral form is consistent with a recent *letter* by Zeman. However, here the constant C_Ω is found to be related to the Kolmogorov constant and is estimated in the range 1.22 – 1.87 for the typical values of the latter constant. A ‘rule’ that

relates spectral transfer times to the eddy turnover time and the time scale for decay of the triple correlations is deduced. A hypothesis for the triple correlation decay rate leads to the spectral law which varies between the ‘ $-5/3$ ’ (without rotation) and ‘ -2 ’ laws (with strong rotation). For intermediate rotation rates, the spectrum varies according to the value of a dimensionless parameter that measures the strength of the rotation wavenumber $k_\Omega = (\Omega^3/\epsilon)^{1/2}$ relative to the wavenumber k . An eddy viscosity is derived with an explicit dependence on the rotation rate.

Girimaji, Sharath S., and Ye Zhou: *Analysis and modeling of subgrid scalar mixing using numerical data*. ICASE Report No. 95-44, May 31, 1995, 31 pages. To be submitted to Physics of Fluids.

Direct numerical simulations (DNS) of passive scalar mixing in isotropic turbulence is used to study, analyze and, subsequently, model the role of small (subgrid) scales in the mixing process. In particular, we attempt to model the dissipation of the large scale (supergrid) scalar fluctuations caused by the subgrid scales by decomposing it into two parts: (i) the effect due to the interaction among the subgrid scales, $\mathcal{E}_\phi^{>>}$; and, (ii) the effect due to interaction between the supergrid and the subgrid scales, $\mathcal{E}_\phi^{><}$. Model comparison with DNS data shows good agreement. This model is expected to find use in the large eddy simulations of scalar mixing and reaction.

Burns, John A., and Belinda B. King: *Representation of feedback operators for hyperbolic systems*. ICASE Report No. 95-45, May 31, 1995, 13 pages. To appear in the “Conference on Computation and Control,” J. Lund, Ed., Burkhöuser, 1995.

We consider the problem of obtaining integral representation of feedback operators for damped hyperbolic control systems. We show that for the wave equation with Kelvin-Voigt damping and non-compact input operator, the feedback gain operator is Hilbert-Schmidt. This result is then used to provide an explicit integral representation for the feedback operator in terms of functional gains. Numerical results are given to illustrate the role that damping plays in the smoothness of these gains.

Speziale, Charles G., Ridha Abid, and Gregory A. Blaisdell: *On the consistency of Reynolds stress turbulence closures with hydrodynamic stability theory*. ICASE Report No. 95-46, August 21, 1995, 22 pages. To be submitted to Physics of Fluids.

The consistency of second-order closure models with results from hydrodynamic stability theory is analyzed for the simplified case of homogeneous turbulence. In a recent study, Speziale, Gatski and MacGiolla Mhuiris [*Phys. Fluids A* 2, 1678, 1990] showed that second-order closures are capable of yielding results that are consistent with hydrodynamic stability theory for the case of homogeneous shear flow in a rotating frame. It is demonstrated in this paper that this success is due to the fact that the stability boundaries for rotating homogeneous shear flow are not dependent on the details of the spatial structure of the disturbances. For those instances where they are – such

as in the case of elliptical flows where the instability mechanism is more subtle – the results are not so favorable. The origins and extent of this modeling problem are examined in detail along with a possible resolution based on Rapid Distortion Theory (RDT) and its implications for turbulence modeling.

Middleton, David: *An executable specification for the message processor in a simple combining network*. ICASE Report No. 95-47, June 12, 1995, 36 pages.

While the primary function of the network in a parallel computer is to communicate data between processors, it is often useful if the network can also perform rudimentary calculations. That is, some simple processing ability in the network itself, particularly for performing parallel prefix computations, can reduce both the volume of data being communicated and the computational load on the processors proper. Unfortunately, typical implementations of such networks require a large fraction of the hardware budget, and so combining networks are viewed as being impractical.

The FFP Machine has such a combining network, and various characteristics of the machine allow a good deal of simplification in the network design. Despite being simple in construction however, the network relies on many subtle details to work correctly. This paper describes an executable model of the network which will serve several purposes. It provides a complete and detailed description of the network which can substantiate its ability to support necessary functions. It provides an environment in which algorithms to be run on the network can be designed and debugged more easily than they would on physical hardware. Finally, it provides the foundation for exploring the design of the message receiving facility which connects the network to the individual processors.

Tidriri, M.D.: *Krylov methods for compressible flows*. ICASE Report No. 95-48, June 30, 1995, 31 pages. To be submitted to Computer Methods in Applied Mechanics and Engineering.

In this paper we investigate the application of Krylov methods to compressible flows, and the effect of implicit boundary conditions on the implicit solution of nonlinear problems. Two defect-correction procedures, namely, Approximate Factorization (AF) for structured grids, and ILU/GMRES for general grids are considered. Also, considered here, is Newton-Krylov matrix-free methods that we combined with the use of mixed discretization schemes in the implicitly defined Jacobian and its preconditioner. Numerical experiments that show the performance of our approaches are then presented.

Bokhari, Shahid H.: *The Linux operating system: An introduction*. ICASE Report No. 95-49, June 30, 1995, 20 pages. IEEE "Computer", Vol. 28, No. 5, August 1995, pp. 74-79.

Linux is a Unix-like operating system for Intel 386/486/Pentium based IBM-PCs and compatibles. The kernel of this operating system was written from scratch by Linus Torvalds and, although copyright by the author, may be freely distributed. A world-wide group of enthusiastic volunteers has collaborated in developing many aspects of Linux on the Internet.

Linux can run the powerful set of compilers and programming tools (the 'GNU' corpus) of the Free Software Foundation, and XFree86, a port of the X Window System from MIT. Most capabilities associated with high performance workstations, such as networking, shared file systems, electronic mail, $\text{\TeX}$, $\text{\LaTeX}$, etc. are freely available for Linux. It can thus transform cheap IBM-PC compatible machines into Unix workstations with considerable capabilities.

The author explains how Linux may be obtained, installed and networked. He also describes some interesting applications for Linux that are freely available. One useful feature of Linux is its ability to coexist with other operating systems. Thus a user who has made an investment in DOS/MSWindows software, may continue running these applications on his machine and install Linux on a separate partition on his existing hard disk. If needed, files from DOS/MSWindows partitions can be accessed by Linux.

The enormous consumer market for IBM-PC compatible machines continually drives down prices of CPU chips, memory, hard disks, CDRoms etc. Linux can convert such machines into powerful workstations that can be used for teaching, research and software development. For professionals who use Unix based workstations at work, Linux permits virtually identical working environments on their personal home machines. For cost conscious educational institutions (especially in developing nations), Linux can create world-class computing environments from cheap, easily maintained, PC clones. Finally, for university students, especially in science and engineering, Linux provides an essentially cost-free path away from DOS into the world of Unix and X Windows.

Banks, David C., and Michael Kelley: *Tracking a turbulent spot in an immersive environment*. ICASE Report No. 95-50, July 5, 1995, 12 pages. Submitted to the 1995 Symposium on Interactive 3D Computer Graphics.

We describe an interactive, immersive 3D system called *Tracktur*, which allows a viewer to track the development of a turbulent flow. *Tracktur* displays time-varying vortex structures extracted from a numerical flow simulation. The user navigates the space and probes the data within a windy 3D landscape. In order to sustain a constant frame rate, we enforce a fixed polygon budget on the geometry. We supplement the interactive system with interactive, hypertext documentation available on the World Wide Web. In actual use by a fluid dynamicist, the system has yielded new insights into the transition to turbulence in a laminar flow.

Banks, David C., and Bart A. Singer: *A predictor-corrector technique for visualizing unsteady flow*. ICASE Report No. 95-51, July 21, 1995, 30 pages. Submitted to IEEE Transactions on Visualization and Computer Graphics.

We present a method for visualizing unsteady flow by displaying its vortices. The vortices are identified by using a vorticity-predictor pressure-corrector scheme that follows vortex cores. The cross-sections of a vortex at each point along the core can be represented by a Fourier series. A vortex can be faithfully reconstructed from the series as a simple quadrilateral mesh, or its reconstruction can be enhanced to indicate helical motion. The mesh can reduce the representation of the flow features by a factor of one thousand or more compared with the volumetric dataset. With this amount of reduction it is possible to implement an interactive system on a graphics workstation to permit a viewer to examine, in three dimensions, the evolution of the vortical structures in a complex, unsteady flow.

Criminale, W.O., D.G. Lasseigne, and T.L. Jackson: *Vortex perturbation dynamics*. ICASE Report No. 95-52, July 17, 1995, 21 pages. Submitted to Physics of Fluids.

An initial value approach is used to examine the dynamics of perturbations introduced into a vortex under strain. Both the basic vortex considered and the perturbations are taken as fully three-dimensional. An explicit solution for the time evolution of the vorticity perturbations is given for arbitrary initial vorticity. Analytical solutions for the resulting velocity components are found when the initial vorticity is assumed to be localized. For more general initial vorticity distributions, the velocity components are determined numerically. It is found that the variation in the radial direction of the initial vorticity disturbance is the most important factor influencing the qualitative behaviour of the solutions. Transient growth in the magnitude of the velocity components is found to be directly attributable to the compactness of the initial vorticity.

Mavriplis, D.J., and V. Venkatakrishnan: *A unified multigrid solver for the Navier-Stokes equations on mixed element meshes*. ICASE Report No. 95-53, July 17, 1995, 26 pages. Submitted to the International Journal of Computational Fluid Dynamics.

A unified multigrid solution technique is presented for solving the Euler and Reynolds-averaged Navier-Stokes equations on unstructured meshes using mixed elements consisting of triangles and quadrilaterals in two dimensions, and of hexahedra, pyramids, prisms and tetrahedra in three dimensions. While the use of mixed elements is by no means a novel idea, the contribution of the paper lies in the formulation of a complete solution technique which can handle structured grids, block structured grids, and unstructured grids of tetrahedra or mixed elements without any modification. This is achieved by discretizing the full Navier-Stokes equations on tetrahedral elements, and the thin layer version of these equations on other types of elements, while using a single edge-based data-structure to construct the discretization over all element types. An agglomeration multigrid algorithm, which naturally handles meshes of any types of elements, is employed to accelerate convergence. An automatic algorithm which reduces the complexity of a given triangular

or tetrahedral mesh by merging candidate triangular or tetrahedral elements into quadrilateral or prismatic elements is also described. The gains in computational efficiency afforded by the use of non-simplicial meshes over fully tetrahedral meshes are demonstrated through several examples.

Tidriri, M.D.: *Mathematical analysis of the Navier-Stokes equations with non standard boundary conditions*. ICASE Report No. 95-54, July 17, 1995, 19 pages. To be submitted to the Journal of Mathematical Analysis and its Applications.

One of the major applications of the Domain Decomposition Time Marching Algorithm is the coupling of the Navier-Stokes systems with Boltzmann equations in order to compute transitional flows. Another important application, is the coupling of a global Navier-Stokes problem with a local one in order to use different modelizations and/or discretizations. Both of these applications involve a global Navier-Stokes system with non standard boundary conditions. The purpose of this work is to prove, using the classical Leray-Schauder theory, that these boundary conditions are admissible and lead to a well posed problem.

Rubinstein, Robert: *Relaxation approximation in the theory of shear turbulence*. ICASE Report No. 95-55, July 21, 1995, 21 pages. To be submitted to Physics of Fluids A.

Leslie's perturbative treatment of the direct interaction approximation for shear turbulence (*Modern Developments in the Theory of Turbulence*, 1972) is applied to derive a time dependent model for the Reynolds stresses. The stresses are decomposed into tensor components which satisfy coupled linear relaxation equations; the present theory therefore differs from phenomenological Reynolds stress closures in which the time derivatives of the stresses are expressed in terms of the stresses themselves. The theory accounts naturally for the time dependence of the Reynolds normal stress ratios in simple shear flow. The distortion of wavenumber space by the mean shear plays a crucial role in this theory.

Haines, Matthew, Piyush Mehrotra, and John Van Rosendale: *SmartFiles: An OO approach to data file interoperability*. ICASE Report No. 95-56, July 21, 1995, 20 pages. To appear in Proceedings of Oopsla95.

Data files for scientific and engineering codes typically consist of a series of raw data values whose description is buried in the programs that interact with these files. In this situation, making even minor changes in the file structure or sharing files between programs (interoperability) can only be done after careful examination of the data files and the I/O statements of the programs interacting with this file. In short, scientific data files lack self-description, and other self-describing data techniques are not always appropriate or useful for scientific data files. By applying an object-oriented methodology to data files, we can add the intelligence required to improve data interoperability and provide an elegant mechanism for supporting complex, evolving, or multidisciplinary applications,

while still supporting legacy codes. As a result, scientists and engineers should be able to share datasets with far greater ease, simplifying multidisciplinary applications and greatly facilitating remote collaboration between scientists.

Ma, Kwan-Liu: *Parallel volume ray-casting for unstructured-grid data on distributed-memory architectures*. ICASE Report No. 95-57, August 21, 1995, 19 pages. To appear in Proceedings of the Parallel Rendering Symposium '95.

As computing technology continues to advance, computational modeling of scientific and engineering problems produces data of increasing complexity: large in size and unstructured in shape. Volume visualization of such data is a challenging problem. This paper proposes a distributed parallel solution that makes ray-casting volume rendering of unstructured-grid data practical. Both the data and the rendering process are distributed among processors. At each processor, ray-casting of local data is performed independent of the other processors. The global image compositing processes, which require inter-processor communication, are overlapped with the local ray-casting processes to achieve maximum parallel efficiency. This algorithm differs from previous ones in four ways: it is completely distributed, less view-dependent, reasonably scalable, and flexible. Without using dynamic load balancing, test results on the Intel Paragon using from two to 128 processors show, on average, about 60% parallel efficiency.

Ueng, S.K., K. Sikorski, and Kwan-Liu Ma: *Fast algorithms for visualizing fluid motion in steady flow on unstructured grids*. ICASE Report No. 95-58, August 21, 1995, 18 pages. To appear in Proceedings of the Visualization '95 Conference.

The plotting of streamlines is an effective way of visualizing fluid motion in steady flows. Additional information about the flowfield, such as local rotation and expansion, can be shown by drawing in the form of a ribbon or tube. In this paper, we present efficient algorithms for the construction of streamlines, streamribbons and streamtubes on unstructured grids. A specialized version of the Runge-Kutta method has been developed to speed up the integration of particle paths. We have also derived closed-form solutions for calculating angular rotation rate and radius to construct streamribbons and streamtubes, respectively. According to our analysis and test results, these formulations are two to four times better in performance than previous numerical methods. As a large number of traces are calculated, the improved performance could be significant.

Iollo, Angelo, Geojoe Kuruvila, and Shlomo Ta'asan: *Pseudo-time method for optimal shape design using the Euler equations*. ICASE Report No. 95-59, September 8, 1995, 23 pages. Submitted to AIAA Journal.

In this paper we exploit a novel idea for the optimization of flows governed by the Euler equations. The algorithm consists of marching on the design hypersurface while improving the

distance to the state and costate hypersurfaces. We consider the problem of matching the pressure distribution to a desired one, subject to the Euler equations, both for subsonic and supersonic flows. The rate of convergence to the minimum for the cases considered is 3 to 4 times slower than that of the analysis problem. Results are given for Ringleb flow and a shockless recompression case.

Venkatakrishnan, V., and D.J. Mavriplis: *Implicit method for the computation of unsteady flows on unstructured grids*. ICASE Report No. 95-60, September 8, 1995, 35 pages. Submitted to the Journal of Computational Physics.

An implicit method for the computation of unsteady flows on unstructured grids is presented. Following a finite difference approximation for the time derivative, the resulting nonlinear system of equations is solved at each time step by using an agglomeration multigrid procedure. The method allows for arbitrarily large time steps and is efficient in terms of computational effort and storage. Inviscid and viscous unsteady flows are computed to validate the procedure. The issue of the mass matrix which arises with vertex-centered finite volume schemes is addressed. The present formulation allows the mass matrix to be inverted indirectly. A mesh point movement and reconnection procedure is described that allows the grids to evolve with the motion of bodies. As an example of flow over bodies in relative motion, flow over a multi-element airfoil system undergoing deployment is computed.

Bokhari, Shahid H.: *Multiphase complete exchange on Paragon, SP2 & CS-2*. ICASE Report No. 95-61, September 25, 1995, 22 pages. Submitted to IEEE Parallel and Distributed Technology.

The overhead of interprocessor communication is a major factor in limiting the performance of parallel computer systems. The *complete exchange* is the severest communication pattern in that it requires each processor to send a distinct message to every other processor. This pattern is at the heart of many important parallel applications. On hypercubes, *multiphase* complete exchange has been developed and shown to provide optimal performance over varying message sizes.

Most commercial multicomputer systems do not have a hypercube interconnect. However they use special purpose hardware and dedicated communication processors to achieve very high performance communication and can be made to *emulate* the hypercube quite well.

Multiphase complete exchange has been implemented on three contemporary parallel architectures: the Intel Paragon, IBM SP2 and Meiko CS-2. The essential features of these machines are described and their basic interprocessor communication overheads are discussed. The performance of multiphase complete exchange is evaluated on each machine. It is shown that the theoretical ideas developed for hypercubes are also applicable in practice to these machines and that multiphase complete exchange can lead to major savings in execution time over traditional solutions.

Sun, Xian-He: *The relation of scalability and execution time*. ICASE Report No. 95-62, September 20, 1995, 24 pages. To be submitted to the 10th International Parallel Processing Symposium.

Scalability has been used extensively as a de facto performance criterion for evaluating parallel algorithms and architectures. However, for many, scalability has theoretical interests only since it does not reveal execution time. In this paper, the relation between scalability and execution time is carefully studied. Results show that the isospeed scalability well characterizes the variation of execution time: smaller scalability leads to larger execution time, the same scalability leads to the same execution time, etc. Three algorithms from scientific computing are implemented on an Intel Paragon and an IBM SP2 parallel computer. Experimental and theoretical results show that scalability is an important, distinct metric for parallel and distributed systems, and may be as important as execution time in a scalable parallel and distributed environment.

Danowitz, Jeffrey S., Saul A. Abarbanel, and Eli Turkel: *A far-field non-reflecting boundary condition for two-dimensional wake flows*. ICASE Report No. 95-63, September 27, 1995, 34 pages. Submitted to the Journal of Computational Physics.

Far-field boundary conditions for external flow problems have been developed based upon long-wave perturbations of linearized flow equations about a steady state far field solution. The boundary improves convergence to steady state in single-grid temporal integration schemes using both regular-time-stepping and local-time-stepping. The far-field boundary may be near the trailing edge of the body which significantly reduces the number of grid points, and therefore the computational time, in the numerical calculation. In addition the solution produced is smoother in the far-field than when using extrapolation conditions. The boundary condition maintains the convergence rate to steady state in schemes utilizing multigrid acceleration.

Joslin, Ronald D., Max D. Gunzburger, R.A. Nicolaides, Gordon Erlebacher, and M. Yousuff Hussaini: *A self-contained, automated methodology for optimal flow control validated for transition delay*. ICASE Report No. 95-64, September 25, 1995, 46 pages. Submitted to the Journal of Fluid Mechanics.

This paper describes a self-contained, automated methodology for flow control along with a validation of the methodology for the problem of boundary layer instability suppression. The objective of control is to match the stress vector along a portion of the boundary to a given vector; instability suppression is achieved by choosing the given vector to be that of a steady base flow, e.g., Blasius boundary layer. Control is effected through the injection or suction of fluid through a single orifice on the boundary. The present approach couples the time-dependent Navier-Stokes system with an adjoint Navier-Stokes system and optimality conditions from which optimal states, i.e., unsteady flow fields, and controls, e.g., actuators, may be determined. The results demonstrate that instability suppression can be achieved without any a priori knowledge of the disturbance, which is significant because other control techniques have required some knowledge of the flow

unsteadiness such as frequencies, instability type, etc. The present methodology can easily be extended to three dimensions and may be directly applied to separation control, re-laminarization, and turbulence control applications using one to many sensors and actuators.

Banks, H.T., Ralph C. Smith, D.E. Brown, Vern L. Metcalf, and R.J. Silcox: *The estimation of material and patch parameters in a PDE-based circular plate model*. ICASE Report No. 95-66, September 27, 1995, 28 pages. Submitted to the Journal of Sound and Vibration.

The estimation of material and patch parameters for a system involving a circular plate, to which piezoceramic patches are bonded, is considered. A partial differential equation (PDE) model for the thin circular plate is used with the passive and active contributions from the patches included in the internal and external bending moments. This model contains piecewise constant parameters describing the density, flexural rigidity, Poisson ratio and Kelvin-Voigt damping for the system as well as patch constants and a coefficient for viscous air damping. Examples demonstrating the estimation of these parameters with experimental acceleration data and a variety of inputs to the experimental plate are presented. By using a physically-derived PDE model to describe the system, parameter sets consistent across experiments are obtained, even when phenomena such as damping due to electric circuits affect the system dynamics.

Blackaby, Nicholas, Andrew Dando, and Philip Hall: *The nonlinear evolution of inviscid Görtler vortices in three-dimensional boundary layers*. ICASE Report No. 95-68, September 27, 1995, 44 pages. Submitted to the Proceedings of the Royal Society A.

The nonlinear development of inviscid Görtler vortices in a three-dimensional boundary layer is considered. We do not follow the classical approach of weakly nonlinear stability problems and consider a mode which has just become unstable. Instead we extend the method of Blackaby, Dando & Hall (1993), which considered the closely related nonlinear development of disturbances in stratified shear flows. The Görtler modes we consider are initially fast growing and we assume, following others, that boundary-layer spreading results in them evolving in a linear fashion until they reach a stage where their amplitudes are large enough and their growth rates have diminished sufficiently so that amplitude equations can be derived using weakly nonlinear and non-equilibrium critical-layer theories. From the work of Blackaby, Dando & Hall (1993) it is apparent, given the range of parameters for the Görtler problem, that there are three possible nonlinear integro-differential evolution equations for the disturbance amplitude. These are a cubic due to viscous effects, a cubic which corresponds to the novel mechanism investigated in this previous paper and a quintic. In this paper we shall concentrate on the two cubic integro-differential equations and in particular on the one due to the novel mechanism as this will be the first to affect a disturbance. It is found that the consideration of a spatial evolution problem as opposed to temporal (as was considered in Blackaby, Dando & Hall 1993) causes a number of significant changes to the evolution equations.

INTERIM REPORTS

Girimaji, Sharath, editor: *The first ICASE/LaRC industry roundtable: Session proceedings*. ICASE Interim Report No. 26, March 2, 1995, 68 pages.

The first "ICASE/LaRC Industry Roundtable" was held on October 3 - 4, 1994, in Williamsburg, Virginia. The main purpose of the Roundtable was to draw attention of ICASE/LaRC scientists to industrial research agendas. The Roundtable was attended by about 200 scientists, of which 30% from NASA Langley; 20% from universities; 17% NASA Langley Contractors (including ICASE personnel); and, the remaining from federal agencies other than NASA Langley. The technical areas covered reflected the major research programs in ICASE and closely associated NASA branches. About 80% of the speakers were from industry. This report is a compilation of the session summaries prepared by the session chairmen.

Macrossan, M.N.: *Some developments of the equilibrium particle simulation method for the direct simulation of compressible flows*. ICASE Interim Report No. 27, June 27, 1995, 33 pages.

The direct simulation Monte Carlo (DSMC) method is the established technique for the simulation of rarefied gas flows. In some flows of engineering interest, such as occur for aero-braking spacecraft in the upper atmosphere, DSMC can become prohibitively expensive in CPU time because some regions of the flow, particularly on the windward side of blunt bodies, become collision dominated. As an alternative to using a hybrid DSMC and continuum gas solver (Euler or Navier-Stokes solver) this work is aimed at making the particle simulation method efficient in the high density regions of the flow. A high density, infinite collision rate limit of DSMC, the Equilibrium Particle Simulation method (EPSM) was proposed some 15 years ago. EPSM is developed here for the flow of a gas consisting of many different species of molecules and is shown to be computationally efficient (compared to DSMC) for high collision rate flows. It thus offers great potential as part of a hybrid DSMC/EPSM code which could handle flows in the transition regime between rarefied gas flows and fully continuum flows. As a first step towards this goal a pure EPSM code is described. The next step of combining DSMC and EPSM is not attempted here but should be straightforward. EPSM and DSMC are applied to Taylor-Couette flow with $Kn = 0.02$ and 0.0133 and $S_w = 3$). Toroidal vortices develop for both methods but some differences are found, as might be expected for the given flow conditions. EPSM appears to be less sensitive to the sequence of random numbers used in the simulation than is DSMC and may also be more dissipative. The question of the origin and the magnitude of the dissipation in EPSM is addressed. It is suggested that this analysis is also relevant to DSMC when the usual accuracy requirements on the cell size and decoupling time step are relaxed in the interests of computational efficiency.

Bokhari, Shahid H.: *Communication overhead on the Intel Paragon, IBM SP2 & Meiko CS-2*. ICASE Interim Report No. 28, September 20, 1995, 19 pages.

Interprocessor communication overhead is a crucial measure of the power of parallel computing systems—its impact can severely limit the performance of parallel programs. This report presents measurements of communication overhead on three contemporary commercial multicomputer systems: the Intel Paragon, the IBM SP2 and the Meiko CS-2. In each case the time to communicate between processors is presented as a function of message length. The time for global synchronization and memory access is discussed. The performance of these machines in emulating hypercubes and executing random pairwise exchanges is also investigated.

It is shown that the interprocessor communication time depends heavily on the specific communication pattern required. These observations contradict the commonly held belief that communication overhead on contemporary machines is independent of the placement of tasks on processors. The information presented in this report permits the evaluation of the efficiency of parallel algorithm implementations against standard baselines.

ICASE COLLOQUIA

April 1, 1995 - September 30, 1995

Name/Affiliation/Title	Date
Kremer, Ulrich, Rice University "Automatic Data Layout for High Performance Fortran"	April 7
Bilger, Robert, The University of Sidney, Australia "Conditional Moment Closure Methods for Complex Kinetics in Turbulent Combustion"	April 7
Kalns, Edgar T., Michigan State University "Scalable Data Redistribution Services for Distributed-Memory Machines"	April 10
Wolkowicz, Henry, University of Waterloo, Canada "A General Framework for Trust Region Subproblems with Applications to Large-Scale Minimization"	April 13
Krantz, Alan, International Institute of Applied System Analysis, Laxenburg, Austria "An Efficient Algorithm for the Hard-Sphere Problem"	April 14
Kraichnan, Robert "Small-Scale Structure of Turbulence"	April 25
Ramesh, Anapathur V., ALGOR, Inc., Pennsylvania "Sensitivity of Transient Solutions of Markov Models"	May 4
McCormick, Stephen, University of Colorado, Boulder "First-Order System Least Squares in Fluid Dynamics"	May 8
Loncaric, Josip, Logis Technologies, Inc. "Systems Engineering and Modular Dextrous Hand (MDH)"	May 15
Woodruff, Stephen, Brown University "Large-Eddy Simulations of Accelerated Turbulent Channel Flow Employing New Subgrid Models"	May 19
Chang, S.C., and C.Y. Loh, NASA Lewis Research Center "The Method of Space-Time Conservation Element and Solution Element - Application to Aeroacoustics Problems"	May 23
Macrossan, Michael, University of Queensland, St. Lucia, Australia "An Application of the Equilibrium Particle Simulation Method to Taylor-Couette Flow"	May 24

Name/Affiliation/Title	Date
Atassi, H.M., University of Notre Dame “Aerodynamics and Aeroacoustics of Nonuniform Flows”	May 26
Knoll, Dana, Idaho National Engineering Laboratory “Newton-Krylov Methods for Low Mach Number Combustion”	June 1
McHugh, P. R., Idaho National Engineering Laboratory “Investigation of Newton-Krylov Algorithms for Solving Incompressible and Low Mach Number Compressible Flow Using Finite Volume Discretization”	June 1
Barber, Thomas, United Technologies Research Center “Turbulence Modeling for Aerospace & Commercial Application”	June 2
Chiueh, Tzi-cker, State University of New York at Stony Brook “Data Compression: A Computer Systems Perspective”	June 6
Hanebutte, Ulf, Intelligent Transportation Systems, Argonne National Laboratory “Parallel Traffic Simulations – An Overview”	June 7
Voke, Peter R., University of Surrey, England “Large-Eddy Simulation of Boundary Layer Bypass Transition Mechanisms”	June 8
Criminale, William, University of Washington “Disturbance Transient Dynamics in Shear Flows”	June 15
Yeung, P.K., Georgia Institute of Technology “Parallel Computations of Turbulent Mixing and Dispersion”	June 19
Reuther, James, RIACS “Practical Aspects of Aerodynamic Shape Optimization Using Adjoint Based Sensitivity Derivatives”	June 20
Nordstrom, Jan, The Aeronautical Research Institute of Sweden “The Use of Characteristic Boundary Conditions for the Navier-Stokes Equations”	June 26
Rao, Jagannatha, University of Houston “New Models for Optimal Truss Topology in Limit Design Based on Unified Elastic/Plastic Analysis”	June 28
McMichael, James, Air Force Office of Scientific Research “AFOSR Research in Turbulence and Internal Flows”	June 29
Banks, David, ICASE “Advanced Illumination Techniques”	June 30

Name/Affiliation/Title	Date
Banks, David, ICASE “Visualizing a Turbulent Spot in a Shear Flow”	July 3
Vermeer, Willem, Delft University of Technology, The Netherlands “Three-Dimensional Visualization of Shock Wave Computations on Unstructured Grids”	July 7
Vaver, Jon, University of Virginia “An Example of Numerical Method Development in the Computational Modeling Process”	July 10
Darmofal, David, University of Michigan “The Importance of Eigenvectors for Local Preconditioners of the Euler Equations”	July 11
Darmofal, David, University of Michigan “Mechanisms and Models of Axisymmetric Vortex Breakdown”	July 13
Guattery, Stephen, Carnegie-Mellon University “On the Performance of Spectral Graph Partitioning Methods”	July 17
Kumar, Vipin, University of Minnesota “Scalable Parallel Algorithms for Sparse Linear Systems”	July 21
Bertoglio, Jean-Pierre, Ecole Centrale de Lyon, France “Towards Spectral Models for Inhomogeneous Turbulence Based on Two-Point Closures”	July 21
Feyock, Stefan, The College of William and Mary “Machine Learning and Knowledge Discovery: An Overview”	July 24
Chan, Tony, University of California, Los Angeles “Multilevel Domain Decomposition and Multigrid Methods for Unstructured Meshes: Algorithms and Theory”	July 25
Gill, Philip, University of California, San Diego “Limited-Storage Quasi-Newton Methods”	July 26
Hanjalic, Kemal, Delft University of Technology, The Netherlands “Exploring and Expanding the Limits of the ‘Equilibrium’ Second-Moment Closures”	July 27
Biegler, Larry, Carnegie-Mellon University “Tailored Process Optimization Based on Reduced Hessian SQP”	July 27
Machiraju, Raghu, The Ohio State University “Spatial Domain Analysis and Control of Volume Reconstruction: A Sampling Theory Approach”	July 28

Name/Affiliation/Title	Date
Piomelli, Ugo, University of Maryland “Subgrid-Scale Energy Transfer in the Wall Layer”	August 1
Sindir, Munir, Rocketdyne Division, Rockwell International “The State-of-the-Practice of the Use of CFD in an Industrial Environment – A Propulsion Company Perspective”	August 4
Smith, Barry, and Lois Curfman McInnes, Argonne National Laboratory “PETSc 2.0 Design and Philosophy and Capabilities – PETSc - An MPI-Based Numerical Library”	August 7
Sorenson, Daniel, Rice University “Implicitly Restarted Arnoldi Methods for Large Scale Eigenvalue Problems”	August 8
Widlund, Olof, Courant Institute of Mathematical Sciences, New York University “Domain Decomposition Methods for Mortar and Spectral Finite Elements”	August 8
Cai, Xiao-Chuan, University of Colorado-Boulder “Overlapping Schwarz Algorithms and Their Application in Flow Problems”	August 9
van de Velde, Eric, California Institute of Technology “Dots Outside the Square”	August 9
Vandewalle, Stefan, California Institute of Technology “Iterative Methods for Ordinary Differential Equations: Waveform Relaxation”	August 10
Fischer, Paul, Brown University “Parallel Complex Geometry Navier-Stokes Computations”	August 11
Horton, Graham, University of Erlangen, Germany “Fluid Stochastic Petri Nets – Formulation and Transient Analysis”	August 11
Kambe, Tsutomu, University of Tokyo “Compression Wave Phenomena Associated with Vorticity Dynamics”	August 15
Gannon, Dennis, Indiana University “HPC++: Data Parallel Constructs for Shared and Distributed Memory ”	August 15
Kesselman, Carl, California Institute of Technology “An Evaluation of CC++ as a Baseline for HPC++”	August 15
Livny, Miron, University of Wisconsin-Madison “The Condor View of Cluster Computing: Past, Present, and Future”	August 16
Laurence, Dominique, Electricite de France, National Laboratory of Hydraulics “Refined Modeling and Validation of Turbulence for Industrial Applications”	August 18

Name/Affiliation/Title	Date
Bataille, Jean, Ecole Centrale de Lyon, France “An Experimental Investigation of the Wall-Turbulent Bubbly Flow Interaction”	August 21
Nieuwstadt, F.T.M., Delft University of Technology, The Netherlands “Large-Eddy Simulation of Axially Rotating and Curved Pipe Flow”	August 22
Ueng, Shyh-Kuang, University of Utah “Out-of-Core Visualization on Unstructured Grids”	August 24
Nguyen, Brian, University of Michigan “Acoustic and Electromagnetic Bicharacteristic Equations Using Upwind Leapfrog: Analyses and Absorbing Boundary Conditions”	August 25
Isler, Sylvia, University of Michigan “Analysis and Visualization of Acoustic Scattered Fields”	August 28
Interrante, Victoria, University of North Carolina, Chapel Hill “Illustrating Transparency – Communicating the Three-Dimensional Shape and Relative Depth of a Layered Transparent Surface Using Sparse Opaque Texture”	August 29
Bokhari, Shahid, University of Engineering & Technology, Lahore, Pakistan “Multiphase Complete Exchange on Paragon, SP2, and CS-2”	August 31
Shivamoggi, Bhimsen, University of Central Florida “Multi-Fractals in Compressible Turbulence”	September 5
Pavarino, Luca, Universita di Pavia, Italy “Domain Decomposition Algorithms for 1) First-Order Systems Least Squares Methods and 2) Spectral Elements for Elasticity”	September 6
Olariu, Stephan, Old Dominion University “Time-Optimal Domain-Specific Querying on Enhanced Meshes”	September 8
Protzel, Peter, FORWISS, Germany “Neural Networks for Control and Classification: Introduction and Application Examples”	September 12
Freund, Roland, AT&T Bell Laboratories “A Lanczos-Type Method for Multiple Starting Vectors and its Use in Large-Scale Matrix Computations”	September 13
Protzel, Peter, FORWISS, Germany “Fuzzy Control: Principles and Application to an Intelligent Driver Assistance System”	September 14
Lewis, Michael, ICASE “What I Saw at Boeing”	September 15

Name/Affiliation/Title	Date
Karr, Charles, and Michael Freeman, University of Alabama “2-D Thrust-Vectoring Nozzle Optimization with a Genetic Algorithm”	September 18
Harris, Vascar, Tuskegee University, Alabama “The Turbulence Generated by an Array of Parallel Rods”	September 19
Gottlieb, David, Brown University “Analysis and Computations of PDE’s Describing Infiltration Processes”	September 19
Dickens, Thomas, Exxon Production Research “Geological Inversion with Layered Diffraction Tomography”	September 29
Sipicic, Slobodan, Wolfram Research, Inc. “Karhunen-Loève Decomposition in Dynamical Modeling — Symbolic Computation Approach”	September 29

ICASE SUMMER ACTIVITIES

The summer program for 1995 included the following visitors:

<u>NAME/AFFILIATION</u>	<u>DATE OF VISIT</u>	<u>AREA OF INTEREST</u>
Abarbanel, Saul Tel-Aviv University, Israel	6/20 - 7/05 8/07 - 9/01 9/19 - 9/29	Applied & Numerical Mathematics
Abboud, Toufic Ecole Polytechnique, France	6/12 - 6/16	Applied & Numerical Mathematics
Agarwal, Ramesh K. Wichita State University	8/07 - 8/10	Applied & Numerical Mathematics
Anderson, Mark Rice University	6/05 - 6/09	Computer Science
Balling, Richard Brigham Young University	6/12 - 6/16	Applied & Numerical Mathematics
Banks, H. Thomas North Carolina State University	5/01 - 5/26	Applied & Numerical Mathematics
Bataille, Jean Laboratoire de Me'canique des Fluides et d'Acoustique, France	8/21 - 8/22	Fluid Mechanics
Bayliss, Alvin Northwestern University	5/17 - 5/19 6/26 - 6/28 7/17 - 7/20 8/02 - 8/03 8/06 - 8/07	Fluid Mechanics
Beckman, Peter Indiana University	8/07 - 8/18	Computer Science
Berger, Stanley University of California Berkeley	7/04 - 8/04 9/11 - 9/15	Fluid Mechanics
Bertoglio, Jean-Pierre Université Claude Bernard, France	7/17 - 7/28	Fluid Mechanics

<u>NAME/AFFILIATION</u>	<u>DATE OF VISIT</u>	<u>AREA OF INTEREST</u>
Biegler, Larry Carnegie-Mellon University	7/26 - 7/27	Applied & Numerical Mathematics
Bloebaum, Christina L. State University of New York at Buffalo	7/24 - 8/25	Applied & Numerical Mathematics
Bokhari, Shahid Pakistan University of Engineering & Technology	6/12 - 9/07	Computer Science
Brandt, Achi Weizmann Institute of Science, Israel	6/26 - 6/27	Applied & Numerical Mathematics
Burns, John Virginia Polytechnic Institute & State University	5/15 - 5/19 8/14 - 8/18	Applied & Numerical Mathematics
Cai, Wei University of California, Santa Barbara	8/14 - 8/18	Applied & Numerical Mathematics
Cai, Xiao-Chaun University of Colorado, Boulder	7/31 - 8/25	Computer Science
Cendes, Zoltan Carnegie-Mellon University	6/12 - 6/16	Applied & Numerical Mathematics
Chakravarthy, Sukumar Metacomp Technologies, Inc.	7/17 - 7/28	Applied & Numerical Mathematics
Chamberlain, Roger Washington University	7/31 - 8/04	Computer Science
Chan, Tony University of California, Los Angeles	7/24 - 7/28	Applied & Numerical Mathematics
Chapman, Barbara University of Vienna, Austria	8/14 - 8/25	Computer Science
Chiueh, Tzi-cker State University of New York Stony Brook	5/15 - 7/14	Computer Science
Chrisochoides, Nikos Syracuse University	8/07 - 8/18	Computer Science
Ciardo, Gianfranco The College of William & Mary	7/31 - 8/04	Computer Science

<u>NAME/AFFILIATION</u>	<u>DATE OF VISIT</u>	<u>AREA OF INTEREST</u>
Clark, Timothy T. Los Alamos National Laboratory	7/17 - 7/28	Fluid Mechanics
Criminale, William O. University of Washington, Seattle	6/01 - 6/16	Fluid Mechanics
Darmofal, David University of Michigan	7/10 - 7/14	Applied & Numerical Mathematics
Deang, Jennifer Virginia Polytechnic Institute & State University	8/07 - 8/18	Applied & Numerical Mathematics
del Rosario, Ricardo Iowa State University	5/22 - 7/28	Applied & Numerical Mathematics
Dikaiakos, Marios University of Washington	7/31 - 8/04	Computer Science
Ditkowski, Adi Tel-Aviv University, Israel	7/03 - 9/01	Applied & Numerical Mathematics
Fischer, Paul Brown University	8/07 - 8/18	Applied & Numerical Mathematics
Follett, William W. Rocketdyne International	6/12 - 6/23	Applied & Numerical Mathematics
Foster, Ian Argonne National Laboratory	8/14 - 8/18	Computer Science
Fox, Geoffrey Syracuse University	8/23 - 8/24	Applied & Numerical Mathematics
Freund, Roland AT&T Bell Laboratories	9/11 - 9/15	Applied & Numerical Mathematics
Gannon, Dennis Indiana University at Bloomington	8/14 - 8/18	Computer Science
Geer, James State University of New York Binghamton	5/29 - 6/02	Applied & Numerical Mathematics

<u>NAME/AFFILIATION</u>	<u>DATE OF VISIT</u>	<u>AREA OF INTEREST</u>
Gill, Philip E. University of California, San Diego	7/26 - 7/28	Applied & Numerical Mathematics
Gottlieb, David Brown University	6/12 - 6/16 7/10 - 7/21 8/14 - 8/25	Applied & Numerical Mathematics
Gottlieb, Jeremy The College of William & Mary	7/31 - 8/11	Computer Science
Grosch, Chester E. Old Dominion University	5/08 - 6/02	Fluid Mechanics
Grunwald, Dirk University of Colorado, Boulder	8/14 - 8/18	Computer Science
Gunzburger, Max Virginia Polytechnic Institute & State University	5/30 - 6/02 6/12 - 6/16	Applied & Numerical Mathematics
Hadid, Ali H. Rocketdyne International	7/10 - 8/04	Fluid Mechanics
Haftka, Rafi University of Florida, Gainesville	6/12 - 6/16	Applied & Numerical Mathematics
Hall, Philip University of Manchester, England	6/05 - 1/24/96	Fluid Mechanics
Hanebutte, Ulf R. Argonne National Laboratory	6/05 - 6/09	Computer Science
Hanjalic, Kemal Delft University of Technology The Netherlands	7/17 - 8/13	Fluid Mechanics
Heidelberger, Philip IBM T.J. Watson Research Center	7/31 - 8/04	Computer Science
Holt, Maurice University of California, Berkeley	9/11 - 9/15	Applied & Numerical Mathematics
Horton, Graham Universitat Erlangen-Nurmberg Federal Republic of Germany	7/26 - 8/25	Computer Science

<u>NAME/AFFILIATION</u>	<u>DATE OF VISIT</u>	<u>AREA OF INTEREST</u>
Howe, Michael Boston University	7/10 - 7/21	Fluid Mechanics
Hu, Fang Old Dominion University	5/08 - 8/04	Fluid Mechanics
Iollo, Angelo Politecnico di Torino, Italy	7/12 - 8/11	Applied & Numerical Mathematics
Jordan, Harry F. University of Colorado, Boulder	7/31 - 8/11	Computer Science
Joseph, Daniel University of Minnesota	6/19 - 6/30	Fluid Mechanics
Kambe, Tsutomu University of Tokyo, Japan	7/17 - 8/11	Fluid Mechanics
Kangro, Urve Carnegie-Mellon University	6/12 - 6/16	Applied & Numerical Mathematics
Kapila, Ashwani Rensselaer Polytechnic Institute	7/03 - 7/14	Fluid Mechanics
Karunaratne, Nilan C. Auburn University	7/31 - 8/25	Computer Science
Kennedy, Ken Rice University	8/23 - 8/24	Computer Science
Kesselman, Carl California Institute of Technology	8/14 - 8/18	Computer Science
Keyes, David Old Dominion University	5/29 - 6/23 7/24 - 9/01	Computer Science
Koelbel, Charles Rice University	6/05 - 6/09 8/21 - 8/24	Computer Science
Kokkolaras, Michael Rice University	5/08 - 6/02	Applied & Numerical Mathematics
Kopriva, David Florida State University	5/08 - 5/19	Applied & Numerical Mathematics

<u>NAME/AFFILIATION</u>	<u>DATE OF VISIT</u>	<u>AREA OF INTEREST</u>
Kozusko, Frank Old Dominion University	5/01 - 7/28	Fluid Mechanics
Kreiss, Heinz-Otto University of California, Los Angeles	9/05 - 9/11	Applied & Numerical Mathematics
Lasseigne, David Glenn Old Dominion University	5/08 - 8/04	Fluid Mechanics
Lee, Jin-Fa Worcester Polytechnic Institute	6/12 - 6/16	Applied & Numerical Mathematics
Leonard, Anthony California Institute of Technology	9/25 - 9/29	Fluid Mechanics
Leutenegger, Scott T. University of Denver	6/19 - 8/11	Computer Science
Liandrat, Jacques M. University of Wisconsin, Madison	9/18 - 10/20	Applied & Numerical Mathematics
Livny, Miron University of Wisconsin, Madison	8/14 - 8/18	Computer Science
Lynch, E. Douglas Rocketdyne International	7/31 - 8/11	Fluid Mechanics
Mahalov, Alex Arizona State University	6/12 - 7/14	Fluid Mechanics
Malony, Al University of Oregon	8/17 - 8/18	Computer Science
Manthey, Joe Old Dominion University	5/08 - 8/18	Fluid Mechanics
McCartin, Brian GMI Engineering & Management Institute	6/12 - 6/16	Applied & Numerical Mathematics
McComb, W. David University of Edinburgh, Scotland	9/11 - 9/27	Fluid Mechanics
McInnes, Lois Curfman Argonne National Laboratory	8/07 - 8/11	Applied & Numerical Mathematics

<u>NAME/AFFILIATION</u>	<u>DATE OF VISIT</u>	<u>AREA OF INTEREST</u>
Mohr, Bernd University of Oregon	8/12 - 8/18	Computer Science
Monk, Peter University of Delaware	6/12 - 6/16	Applied & Numerical Mathematics
Nguyen, Brian University of Michigan, Ann Arbor	7/06 - 9/01	Applied & Numerical Mathematics
Nicol, David The College of William & Mary	7/31 - 8/11	Computer Science
Nicolaides, R. A. Carnegie-Mellon University	5/30 - 6/01 6/12 - 6/16 7/12 - 7/28	Applied & Numerical Mathematics
Nieuwstadt, F.T.M. Delft University of Technology The Netherlands	8/21 - 8/23	Fluid Mechanics
O'Hallaron, David Carnegie-Mellon University	7/31 - 8/04 8/22 - 8/23	Computer Science
Oliker, Vladimir Emory University	6/12 - 6/16	Applied & Numerical Mathematics
Ozturan, Can Rensselaer Polytechnic Institute	7/31 - 8/18	Computer Science
Papageorgiou, Demetrius New Jersey Institute of Technology	5/29 - 6/16	Fluid Mechanics
Pavarino, Luca F. Universita di Pavia, Italy	7/24 - 9/08	Applied & Numerical Mathematics
Petropoulos, Peter Southern Methodist University	6/12 - 6/20	Applied & Numerical Mathematics
Pothen, Alex Old Dominion University	5/29 - 8/25	Computer Science
Protzel, Peter FORWISS, Germany	9/05 - 9/19	Computer Science

<u>NAME/AFFILIATION</u>	<u>DATE OF VISIT</u>	<u>AREA OF INTEREST</u>
Rao, Jagannatha University of Houston	6/26 - 6/30	Applied & Numerical Mathematics
Roe, Kevin Syracuse University	5/22 - 8/20	Computer Science
Roe, Philip University of Michigan, Ann Arbor	6/26 - 7/07 7/17 - 8/11	Applied & Numerical Mathematics
Sameh, Ahmed University of Minnesota	6/12 - 6/16	Computer Science
Sarkar, Sutanu University of California, San Diego	7/17 - 7/28	Fluid Mechanics
Schreiber, Rob RIACS	8/23 - 8/25	Computer Science
Schwetman, Herb Mesquite Software, Inc.	8/03 - 8/04	Computer Science
Shore, Robert Hanscom Air Force Base	6/12 - 6/16	Applied & Numerical Mathematics
Shu, Chi-Wang Brown University	5/22 - 6/02 7/24 - 8/04 9/11 - 9/22	Applied & Numerical Mathematics
Slechta-Shah, Patricia Boston University	6/19 - 9/08	Fluid Mechanics
Smith, Barry Argonne National Laboratory	8/07 - 8/09	Applied & Numerical Mathematics
Smith, Ralph Iowa State University	5/15 - 7/07	Applied & Numerical Mathematics
Somani, Arun The University of Washington, Seattle	8/21 - 12/15	Computer Science
Sorensen, Daniel Rice University	7/17 - 8/11	Applied & Numerical Mathematics
Speziale, Charles G. Boston University	5/22 - 5/26 7/10 - 7/21 9/18 - 9/22	Fluid Mechanics

<u>NAME/AFFILIATION</u>	<u>DATE OF VISIT</u>	<u>AREA OF INTEREST</u>
Sun, Xian-He Louisiana State University	7/10 - 8/11	Computer Science
Ta'asan, Shlomo Carnegie-Mellon University	5/08 - 5/12 6/22 - 6/30 7/31 - 8/25	Applied & Numerical Mathematics
Taflove, Allen Northwestern University	6/12 - 6/16	Applied & Numerical Mathematics
Tal-Ezer, Hillel Tel-Aviv University, Israel	6/19 - 7/07	Applied & Numerical Mathematics
Tam, Christopher Florida State University	5/15 - 5/19 6/26 - 6/30	Applied & Numerical Mathematics
Thangam, Siva Stevens Institute of Technology	6/12 - 7/07	Fluid Mechanics
Ting, Lu New York University	6/05 - 6/09 7/24 - 8/04	Fluid Mechanics
Trivedi, Kishor Duke University	7/31 - 8/11	Computer Science
Tuecke, Steven Argonne National Laboratory	8/14 - 8/18	Computer Science
Turkel, Eli Tel-Aviv University	6/12 - 6/16 7/03 - 8/25 9/18 - 9/20	Applied & Numerical Mathematics
Ueng, Shyh-Kuang University of Utah	6/05 - 8/25	Computer Science
Ulrey, Michael L. Boeing	8/07 - 8/09	Computer Science
van de Velde, Eric California Institute of Technology	8/07 - 8/11	Applied & Numerical Mathematics
van Leer, Bram The University of Michigan, Ann Arbor	5/01 - 5/06 6/06 - 6/09 7/05 - 7/14	Applied & Numerical Mathematics

<u>NAME/AFFILIATION</u>	<u>DATE OF VISIT</u>	<u>AREA OF INTEREST</u>
Vandewalle, Stefan California Institute of Technology	8/07 - 8/11	Applied & Numerical Mathematics
Voke, Peter R. University of Surrey, England	6/05 - 6/16	Fluid Mechanics
Widlund, Olof New York University	8/07 - 8/11	Computer Science
Woodruff, Stephen Brown University	7/24 - 9/01	Fluid Mechanics
Wu, Jie-Zhi University of Tennessee Space Institute	7/03 - 7/28	Fluid Mechanics
Xu, Jinchao Pennsylvania State University	8/28 - 9/22	Applied & Numerical Mathematics
Yeung, Pui-Kuen Georgia Institute of Technology	6/12 - 6/23	Fluid Mechanics
Younis, Bassam A. City University, England	6/01 - 9/01	Fluid Mechanics
Zemach, Charles Los Alamos National Laboratory	7/10 - 7/21	Fluid Mechanics
Zhang-Sun, Hong Clemson University	7/10 - 8/11	Applied & Numerical Mathematics
Zima, Hans University of Vienna, Austria	8/14 - 9/15	Computer Science
Zurigat, Yousef H. University of Jordan	6/12 - 8/11	Fluid Mechanics

OTHER ACTIVITIES

A series of forums were organized at ICASE during the summer period. Information was exchanged on the latest techniques, both computational and theoretical, along with potential and practical applications. Members from academia, industry, and government labs were represented.

Assessment of Advanced Hardware and Software Architectures

A workshop on the Assessment of Advanced Hardware and Software Architectures, organized by David Nicol, was held during August 1995. The purpose of the workshop was to communicate the various approaches being explored, and to foster future collaborative efforts. The emphasis was on emerging assessment technology suitable for modeling the execution of scientific programs on high performance parallel computers. Advanced modeling concepts, advanced modeling problems, algorithmic aspects, and emerging tools were discussed. Presentations were given on parallel simulation tools, simulation problems in modeling optical interconnection networks, functional algorithm simulation, parallel simulation of execution driven architectural simulation, fluid stochastic petri nets, and parallel techniques for generating and analyzing large discrete state-spaces (such as are generated in tools modeling computer and communication systems). There were nine participants from academia and industry.

Electromagnetics

A summer forum on computational electromagnetics was organized at ICASE by Roy Nicolaidis of Carnegie Mellon University, and held during the week of June 16, 1995. Computational electromagnetics is a rapidly expanding discipline, particularly in its mathematical aspects. The presentations covered the full range of high frequency electromagnetic computations, including radar cross sections, microwave devices and circuits. Contributions from the various speakers covered FDTD techniques for structured and unstructured meshes, finite element approaches and error estimates, industrial applications, and integral equation and boundary element methods. In addition, there were talks on electromagnetics for materials with memory, antenna synthesis, and asymptotics for high frequency problems.

There were also several talks which covered absorbing boundary conditions, integral equation approaches, differential equation approaches and future issues in computational electromagnetics. The workshop was very successful and was a profitable experience for all 11 participants.

Parallel Numerical Algorithms

A workshop on Parallel Numerical Algorithms, organized by David Keyes, was held during August 1995. Emphasis was placed on iterative domain decomposition, a natural form of data parallelism

for computational partial differential equations. Both algorithmic and implementational aspects were considered, together with the related areas of eigenvalue problems and waveform relaxation for time-dependent problems.

The theoretical framework of domain decomposition algorithms has been in place for nearly a decade. In common with elementary relaxation methods and multigrid, they are subspace correction methods. Contemporary efforts, presented and pursued at ICASE, include extending the theory to more general discretizations (nonnested unstructured grids, p -type finite elements) and more general formulations (coupled systems and nonlinear systems), while also seeking better implementations for the inevitable coarse-grid problem, which is the bottleneck of the parallelization.

A spontaneous offshoot of the parallel algorithms concentration, organized by Paul Fischer of Brown University, was a roundtable on computational science curricula and syllabi for graduate courses in parallel algorithms. There were 16 participants.

Turbulence

A forum on turbulence modeling organized by Robert Rubinstein was held during the week of July 10. Presentations by theorists, modelers, and users of turbulence models were juxtaposed to encourage interaction between these often disparate groups of researchers. The purpose of the forum was to air differences of opinion on objectives and methodologies, discover common ground, and decide how the entire community can work more effectively together. Presentations were given on analytical theories, two point models for inhomogeneous turbulence, continuum mechanical methods in single point modeling, and the requirements of the aerodynamics and acoustics communities. The recent development of time-dependent Reynolds averaged models has blurred their distinction with some of the subgrid-scale models currently used in large-eddy simulations. Issues relating to their application to unsteady and nonequilibrium problems were addressed in the final session. There were 12 participants.

Multithreading and HPC++

A workshop on HPC++ and multithreading environments, organized by Piyush Mehrotra, was held during the week of August 14 - 18, 1995. The workshop began with a PORTS meeting, an ongoing series of meetings which is attempting to define a standard interface for multithreading environments. Several speakers described their approach for supporting multithreading efficiently on a wide variety of target architectures.

HPC++ consists of extensions to C++ for parallel and distributed computing currently under development by a group of researchers from universities, research labs and industry. Several speakers gave their vision of HPC++. There followed discussions on how to integrate these different views and extend the current language to support data parallel applications. There were 20 attendees.

High Performance Fortran

A mini-forum on High Performance Fortran (HPF) was organized by Piyush Mehrotra on August 22-23, 1995. HPF is the set of extensions to Fortran 90 for porting data parallel applications to parallel machines. The first day of the mini-forum consisted of reports by three compiler vendors on the status of their HPF compilers. A couple of users then presented their experiences with these and other compilers on their HPF codes. The second day started out with a talk on HPF and its relationship to emerging technologies such as the World Wide Web. This was followed by open discussion on the future of HPF and in particular on how to increase the acceptability of HPF in the user community. The mini-forum was a success in providing the attendees, in particular, the scientists and engineers from NASA, with the current status of the language and the compiler. There were 25 attendees.

Visualizing Time-Varying Data

On September 18-19, 1995 ICASE and NASA LaRC co-sponsored a Symposium on Visualizing Time-Varying Data at the Fort Magruder Inn in Williamsburg, VA. The objective of this Symposium was to bring the producers of time-varying data-sets together with visualization specialists to assess open issues in the field, present new solutions, and encourage collaborative problem-solving.

Conference attendees delivered peer-reviewed technical papers and presented informal videotapes of work in progress. Participants gave live demonstrations of new visualization software systems that are being developed by industry, academia, and government labs. There were 68 attendees, and a NASA Conference Proceedings will be published.

ICASE STAFF

I. ADMINISTRATIVE

M. Yousuff Hussaini, Director. Ph.D., Mechanical Engineering, University of California, 1970.

Linda T. Johnson, Office and Financial Administrator

Etta M. Blair, Accounting Supervisor

Barbara A. Cardasis, Administrative Secretary

Shannon L. Keeter, Technical Publications Secretary

Rachel A. Lomas, Payroll and Accounting Clerk

Shelly D. Millen, Executive Secretary/Visitor Coordinator

Emily N. Todd, Conference Manager

Gwendolyn W. Wesson, Contract Accounting Clerk

Leon M. Clancy, System Manager

Bryan K. Hess, Assistant System Manager (Beginning June 1995)

Avik Banerjee, System Operator

II. SCIENCE COUNCIL

Ivo Babuska, Professor, Institute for Physical Science & Technology, University of Maryland.

Geoffrey Fox, Director, Northeast Parallel Architectural Center, Syracuse University.

Dennis Gannon, Professor, Center for Innovative Computer Applications, Indiana University.

Ashwani Kapila, Professor, Department of Mathematics and Science, Rensselaer Polytechnic Institute.

James P. Kendall, Jet Propulsion Laboratory.

Heinz-Otto Kreiss, Professor, Department of Mathematics, University of California at Los Angeles.

Sanjoy Mitter, Professor of Electrical Engineering, Massachusetts Institute of Technology.

Steven A. Orszag, Professor, Program in Applied & Computational Mathematics, Princeton University.

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III. RESEARCH FELLOWS

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